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TECHNICAL PROGRESS REPORT

Contract E(11-1)-3084

A Combined Macroscopic and Microscopic Approach to the Fracture of Metals

Period: July 1974 - June 1975

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Outline of Work in Progress During Period July 1974 - June 1975

1. Fracture processes at a macroscopic crack tip
2. Theoretical studies on the inception of ductile rupture
3. Diffusive rupture processes
4. Boundary and particle strengthening in steels
5. Fracture surface characterization

Summary of Accomplishments and Work in Progress

Major studies have been completed on 1) the microscale fracture conditions for the brittle and ductile fracture initiation modes at a macroscopic crack tip, 2) the formulation of dilational plasticity constitutive relations for void containing materials as applied to the inception of ductile rupture, 3) cavity growth during diffusive rupture processes as encountered in creep rupture at low stress but high temperature, and 4) particle and boundary strengthening mechanisms in carbon steels.

In addition, work has continued on the crack tip modelling by finite elements and ductile void growth near a crack tip.

Five Ph.D. theses were completed during this contract period.

1. Fracture Processes at a Macroscopic Crack Tip

a) Crack tip modelling by finite elements

Solutions have been obtained by large deformation plane strain finite elements for a crack blunting smoothly in an elastic-plastic material. As described in the Technical Progress Report for June 1973 to June 1974, the boundary conditions for the circle of material with center at the crack tip are obtained from previous larger scale finite element results with small geometry change assumptions. The solutions obtained are for non-hardening (hardening exponent zero), and power hardening (exponents 0.1 and 0.2) plastic behavior. Consequently detailed records of true stress, true strain, and total equivalent plastic strain everywhere in the near tip region are available. Due to the similarity between each solution obtained after an increment of deformation, many data points are available even over size scales of order of one crack opening displacement.

An example of the results available is provided by the calculated maximum achievable stress levels ahead of the crack tip. These are 2.9 σ_o, 3.5 σ_o, and 4.6 σ_o for hardening exponents of 0, .1, and .2, respectively, where σ_o is the initial yield stress. The crack tip opening displacement can also be estimated accurately from the large-strain program. The value is, for a non-hardening material in small scale yielding at stress intensity K, .62 $K^2/E\sigma_o$, where E is Young's modulus. The numerical factor reduces to .41 and .29 for hardening exponents of .1 and .2, respectively.

Such stress and deformation analyses of the crack tip region are of great value for the interelation between macroscopic fracture toughness values and microscale mechanisms of cleavage and rupture. Indeed, their utility is demonstrated by the recent studies under this contract on radiation embrittlement in a pressure-vessel steel and on compositional effects on the fracture toughness of spheroidized carbon steels. The recently obtained finite element results are presently being reduced to a presentable form, and a report is expected by late summer.

(Staff: R. M. McMeeking, D. M. Parks, and J. R. Rice)

b) Microscale fracture mechanisms at a macroscopic crack tip in spheroidized steels

A phase of this part of the program was completed this year; it deals with the correlation of fracture toughness parameters and microstructural parameters of spheroidized carbon steels at low temperatures. It establishes the conditions of brittle fracture initiation at a macroscopic crack tip and the transition from cleavage to fibrous fracture initiation.

The experimental procedure consisted of determining the fracture toughness parameter K_{IC} of circumferentially notched and pre-cracked tensile specimens of four carbon steels (0.13 - 1.46%C) in the temperature range -196° to -110°C. The steels were heat treated to produce a range of cementite particle sizes and spacings which were measured by electron microscopy.

The most significant results were as follows:

1) While the overall fracture mode was brittle for all specimens at all temperatures, the fracture initiation at the macroscopic crack tip changed from a cleavage mechanism to a ductile mechanism as either the temperature of testing was increased for a particular steel microstructure or as the yield strength of the specimens was decreased at constant testing temperature. In both cases, the fracture initiation occurs at the carbide particles.

2) In the case of cleavage initiated fracture, the fracture toughness parameter, K_{IC}, is related to a critical cleavage stress, σ_f^*, achieved over a characteristic microstructural distance, X. At very low temperatures, when σ_f^* is of size comparable to or smaller than the yield stress, this reduces to

$$K_{IC} = \sigma_f^* \sqrt{2 \pi X} \quad ;$$

as temperature increases, and yield strength decreases, the predicted value increases in accordance with the Ritchie, Knott and Rice model. In our materials, it was found that σ_f^* is the critical cleavage propagation stress:

$$\sigma_f^* = \left[\frac{4E\gamma}{\pi(1 - \nu)^2 d} \right]^{1/2}$$

where d is the carbide thickness, and γ is the effective surface energy of the ferrite. The characteristic distance, X, is of the order of 1 - 2 grain sizes.

3) Fibrous initiation occurs when the stress intensification ahead of the crack tip is insufficient to attain the critical cleavage stress. The localized high strains cause void initiation at particles and coalescence over a planar nearest neighbor distance Δ_2. The approximate values of the fracture toughness parameter, K_{IC}, can be predicted through the relation for the crack opening displacement:

$$\delta_t = 0.5 \frac{K_{IC}^2}{E\sigma_y} \quad ,$$

where σ_y is the yield strength and $\delta_t \simeq \Delta_2$ at the onset of ductile rupture.

4) In general, K_{IC}, decreases with decreasing mean-free-path between particles, at constant particle size, i.e. with increasing volume fraction of the carbide; but K_{IC} increases with decreasing carbide particle size at constant composition.

A Ph.D. thesis was submitted by S. Rawal on the basis of this work.

(Staff: J. Gurland, S. Rawal, and J. R. Rice)

c) Studies of ductile void growth near a crack tip

In many cases of ductile rupture, voids nucleate from inclusions at a comparatively early stage in the deformation and grow stably to terminal coalescence, either with neighboring voids or with the main crack. Slip-line field solutions for strains in crack tip blunting are being used together with models for the growth of isolated voids, to estimate the amount and positional dependence of hole growth near a crack tip. These studies extend earlier work by Rice and Johnson, and involve particular attention to void growth off the plane of the crack and its possible relation to ductile fracture propagation in a zig-zag mode.

Void growth and crack blunting eventually reduce the material between a crack and a void to a small ligament of highly strained material. It is assumed in the model that a coalescence instability occurs when this ligament becomes comparable in size to half the largest void dimension. The postulated mechanism, when analyzed with the Rice and Johnson slip line field, causes voids between angles of 45° above and below the crack line ahead of the crack to coalesce with the crack. Elsewhere the void will not coalesce with the crack, but be deformed into a narrow ellipsoid with major axis parallel to the crack. These will lie within one quarter of a crack width on either side of the crack.

For voids which do coalesce with the crack, the crack opening width to cause coalescence rises with increasing magnitude of the angle between the crack line and the line from the void to the crack tip in the undeformed configuration. If this mechanism operates as a ductile crack advance mechanism, then the crack will advance on its original crack line. This seems to contradict the observed zig-zag of stable crack advance under ductile conditions, and suggests that other causes must be found for it.

Currently the investigation is being extended to a crack which blunts with sharp vertices. Slip line solutions are already in existence and the results may shed some light on whether a crack with sharp vertices induces different void growth and coalescence behavior due to the creation of new surface which occurs at the sharp vertices.

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

2. Theoretical Studies on the Inception of Ductile Rupture

A major study has been completed on the formulation of dilational plasticity constitutive relations for void-containing materials. Work reported in prior years focused on the effect of void volume fraction and, within limits, void shape on the overall stress-strain behavior of such materials. This included particularly the dependence of deformation on the mean tensile stress, in general states of combined stressing.

Studies in the current reporting period have incorporated progressive void nucleation, by particle failure, into the constitutive description. This has been done for two cases, chosen as representative of extremes in nucleation behavior: the Gurland model of a plastic-strain dependent volume fraction of failed particles, and the Argon model of nucleation by attainment of a critical tensile stress on the particle-matrix interface. The latter case includes an account of the statistics of the particle distribution in setting the range of stresses over which the particles fail. The constitutive relations that result, incorporating both growth of existing voids and nucleation of new voids, provide a basis for prediction of the inception of ductile rupture.

This appears as a deformation instability, at which the progressive hardening of the ductile matrix material is just balanced by the overall softening due to porosity increase by void nucleation and growth. Thus far, the formulation has been applied primarily to cases of homogeneous deformation. These lead to results that are suggestive of observed ductile fracture behavior; e.g., plane strain tensile ductility is found to be reduced considerably from that for axi-symmetric tension. But it is felt that the full potential of the approach will be realized only when the new constitutive descriptions are incorporated within large-strain finite element codes, so that necking and other cases of inhomogeneous deformation prior to fracture can be properly treated. Such studies are to be proposed for continuing work in the coming year.

(Staff: A. E. Gurson and J. R. Rice)

3. Diffusive Rupture Processes

The focus of work in this area is on creep rupture in a range of high temperature but low stress for which diffusion is the dominant mechanism of inelastic deformation. To examine first a case representing an opposite extreme from that previously studied, attention was directed to a grain boundary cavity growing at a sufficiently rapid rate for its shape to be long and crack-like. This occurs when the time over which the cavity length changes appreciably is short by comparison to relaxation times for surface diffusion. The mechanism of growth is the diffusion of matter from the cavity surfaces to positions along the non-cavitated portion of grain boundary, where atoms are deposited to the adjoining crystals under action of the applied stress.

When adjacent sources of matter (e.g., other rupture cavities) are close at hand, the grains move apart as rigid bodies. This causes a uniform gradient in the grain boundary diffusion flux, and the net applied stress necessary to make the cavity grow at some speed V is found to take the form

$$\sigma = \alpha V^{1/3} + \beta V^{2/3}.$$

Here α, β depend on surface and grain boundary diffusion parameters and, also, on the length and spacing of the cavities. By contrast to the classical Hull-Rimmer case, for which it is assumed that the cavities have spherical (equilibrium) shapes, there is no apparent threshold stress level, and a different variation of speed with stress is implied at higher stress levels.

A second limiting case, for which the void is also assumed to be flat and cracklike, is that in which neighboring matter sources are far removed, and the diffusive flow of matter from the cavity surfaces must be accommodated by elastic deformation of the adjacent grains. This involves a difficult coupled elasticity-diffusion problem, which has been solved numerically to yield the stress needed to drive the crack at any speed. This stress is only slightly speed dependent, and the essential conclusion is that there is a limiting stress level, equal approximately to 1.7 times the critical Griffith stress for an atomistically sharp grain boundary crack, above which very rapid diffusive growth occurs, even in the absence of nearby matter sources.

A start has also been made on finding some solutions intermediate between the flat, crack-like, non-equilibrium shape, appropriate to rapid growth, and the spherical, quasi-equilibrium shape for slow growth. For example, a class of self-similar cavity shapes is being studied, for which all dimensions vary as the quarter power of time. By appropriate choice of parameters, this may be made to coincide with either of the limiting cases.

(Staff: T-j. Chuang, K. Kagawa, and J. R. Rice)

4. Boundary and Particle Strengthening in Steels

A part of this program was completed this year by attaining it's objective, namely to account for the separate contributions of particles, subgrain boundaries, and grain boundaries to the flow stress of carbon steels on the basis of new experimental data and current dislocation-based theories. Essentially, the results show that the particles by themselves have only a small effect on the yield strength, but can make a large contribution to strain hardening whereas subgrain boundaries have a determining influence in all ranges of strain. A more detailed summary follows:

The combined effects of cementite particles, grain boundaries, and subgrain boundaries on the room temperature yielding and strain-hardening behavior of spheroidized plain carbon steels were investigated.

The spheroidized structures were obtained by austenitizing and quenching, followed by either tempering at temperatures just below the A_1 temperature or thermal cycling about the A_1 temperature. Electron microscopy revealed a subgrain network connecting the cementite particles in the steels which were spheroidized by quenching and tempering, and a subgrain-free cementite particle distribution in large ferrite grains in the steels which were spheroidized by the quench-and-cycle procedure. The two different microstructural types were designated as POB, particles on boundaries, and PIB, particles inside boundaries, respectively.

The mean subgrain size, L, in POB specimens was shown to be related to the particle radius, r, by

$$L = 0.22 + 1.63 \frac{r}{f^{1/2}}, \quad \mu m$$

where f is the volume fraction of cementite. This correlation was seen to be in reasonable accord with the Zener-Gladman theory for grain growth, modified for the present case where all second-phase particles are assumed to lie on the boundaries.

The subgrain network in the POB specimens precludes the operation of the Orowan yielding mechanism. The effect of the cementite particles on the lower yield stress is believed to be indirect in that it is the subgrain size, stabilized by the particles, which governs the yield stress. The Hall-Petch relation describing this behavior is

$$\sigma_y = 9.5 + 1.33 \lambda_{\ell,p}^{-1/2}, \quad kgf/mm^2$$

where $\lambda_{\ell,p}$ is the subgrain size corrected for the presence of the second phase $\{\lambda_{\ell,p} = L(1 - f)\}$. The correlations of yield stress with interparticle distance, previously observed in the literature, are understood from the proportionality between the subgrain size and the interparticle spacing for a given volume fraction of cementite.

In the PIB specimens the cementite particles are dispersed in a ferrite matrix of grain size appreciably larger than the mean free path between the particles. The lower yield stress could not be accounted for by either the Orowan or the Ansell-Lenel theory. In these steels, the role of cementite particles was found to be minimal and the lower yield stress to be predominantly controlled by the ferrite grain size, λ_g, via the Hall-Petch relation

$$\sigma_y = 12.4 + 1.87\ \lambda_g^{-1/2}\ ,\ \mathrm{kgf/mm^2}$$

The intraboundary particles contribute only a small strain-hardening term which increases the value of the friction stress (12.4 $\mathrm{kgf/mm^2}$) over that associated with grain boundary strengthening alone (8.8 ± 0.8 $\mathrm{kgf/mm^2}$).

The strain-hardening behavior of the spheroidized steels was examined in terms of recent continuum and quasi-continuum models based on the requirement that continuity be maintained at various boundaries in the two-phase polycrystal . For plastic strains up to 3.5% the increase in the flow stress appears to be composed of contributions arising from (i) dislocations stored in the material for a) statistical and b) geometrical reasons and (ii) an average back stress due to the presence of the unrelaxed plastic strain discontinuity between the matrix and the particles. The latter contribution, which is a large fraction of the total strain-hardening increment, increases rapidly with strain up to a plastic strain of 3.5% and remains approximately constant thereafter. The attainment of the maximum value of the back stress corresponds to the observed transition in the overall strain-hardening rate ("double-n" behavior). The experimentally determined components of the hardening increment, due to the geometrically necessary dislocations, agree well with the predictions of Ashby's theory for the hardening increments in polycrystal (POB) and dispersion strengthened (PIB) materials.

At strains greater than 3.5%, the average back stress remains approximately constant and the geometrically necessary dislocation density increases only slightly with strain. This indicates a deviation from Ashby's theory which predicts a continuous increase of this dislocation population with strain. The strain-hardening increments at these strain levels therefore appear to be controlled mainly by the increase in the statistical dislocation population.

A Ph.D. thesis was submitted by L. Anand on the basis of this work.

(Staff: L. Anand and J. Gurland)

5. Metallographic Characterization of Fracture Surface Profiles on Sectioning Planes

A limited effort was continued to be devoted to this topic. It is the purpose of this work to investigate certain metallurgical and geometrical features of fracture surfaces by means of measurements on metallographic sections showing a fracture surface profile. The features of interest are the relative concentrations of the microstructural constituents on the fracture surface and fracture surface traces, the roughness of the surface traces, and the curvature of the surface traces. Severe limitations are imposed on the three-dimensional interpretation of the two-dimensional measurements by the lack of randomness of the orientations of the surfaces and of the sectioning planes.

The quantitative measurements were applied to brittle and ductile fracture surfaces of Charpy V-notch impact specimens of a 1018 steel. The results are as follows: 1) the ductile fracture path favors the ferrite at the expense of pearlite, but the brittle fracture path does not appear to discriminate between the two constituents. 2) The planar roughness of the two types of fracture surfaces is not significantly different. 3) The average of the local planar curvature of the surfaces may be a significant parameter.

(Staff: J. Gurland)

Technical Reports

COO-3084-29 Progress Report, July 1974

COO-3084-30 L. B. Freund, The Motion of a Crack in an Elastic Solid Subjected to General Loading, August 1974.

COO-3084-31 L. Anand and J. Gurland, The Relationship Between the Size of Cementite Particles and the Subgrain Size in Spheroidize-Annealed Martensites of Steels, August 1974.

COO-3084-32 T. J. Chuang, Models of Intergranular Creep Crack Growth by Coupled Crack Surface and Grain Boundary Diffusion, January 1975.

COO-3084-33 J. Pickens and J. Gurland, Metallographic Characterization of Fracture Surface Profiles on Sectioning Planes, December 1974.

COO-3084-34 D. M. Parks, Interpretation of Irradiation Effects on the Fracture Toughness of a Pressure Vessel Steel in Terms of Crack Tip Stress Analysis, January 1975.

COO-3084-35 L. Anand and J. Gurland, Effect of Internal Boundaries on the Yield Strength of Spheroidized Steels, April 1975.

COO-3084-36 L. Anand, Combined Effects of Particle and Boundary Strengthening in Spheroidized Steels, May 1975.

COO-3084-37 L. Anand and J. Gurland, Strain Hardening of Spheroidized Steels, May 1975.

Publications

L. B. Freund, The Motion of a Crack in an Elastic Solid Subjected to General Loading; Proc. Int. Conference on Dynamic Crack Propagation; G. C. Sih editor, Nordhoff Int. Publ., Leyden, Holland, 1974, p. 553.

L. Anand and J. Gurland, The Relationship Between the Size of Cementite Particles and the Subgrain Size in Quenched and Tempered Steels, Metallurgical Trans. (1975) 6A, p. 928-931.

J. Pickens and J. Gurland, Metallographic Characterization of Fracture Surface Profiles on Sectioning Planes, Proceedings, Fourth International Congress for Stereology, Intern. Soc. for Stereology, In Press.

*P. C. Jindal and J. Gurland, Relation of Hardness and Microstructure of Tempered and Spheroidized Carbon Steels, Metallurgical Trans., 5 (1974), p. 1649.

*J. Gurland, Fracture of Metal-Matrix Particulate Composites--A Review, in Composite Materials, Vol. 5, Fatigue and Fracture, L. J. Brautman and R. H. Krock, Editors, Academic Press, Inc. New York (1974), p. 45-90.

D. M. Parks, Interpretation of Irradiation Effects on the Fracture Toughness of a Pressure Vessel Steel in Terms of Crack Tip Stress Analysis, ASME Journal of Engineering Materials and Technology, to be published.

* Listed as "in press" in previous progress reports.

Theses

L. Anand, Ph.D. Thesis: "Combined Effects of Particle and Boundary Strengthening in Spheroidized Steels," May 1975.

T. J. Chuang, Ph.D. Thesis: "Models of Intergranular Creep Crack Growth by Coupled Crack Surface and Grain Boundary Diffusion," November 1974.

A. E. Gurson, Ph.D. Thesis: "Plastic Flow and Fracture Behavior of Ductile Materials, Incorporating Void Nucleation, Growth, and Interaction," May 1975.

D. M. Parks, Ph.D. Thesis: "Some Problems in Elastic-Plastic Finite-Element Analysis of Cracks," May 1975.

S. P. Rawal, Ph.D. Thesis: "The Relationship Between Fracture Toughness and Microstructural Parameters for Spheroidized Carbon Steels," May 1975.

Oral Presentations

J. R. Rice presented seminar talks on research topics related to this contract at:

Battelle Memorial Institute/Ohio State University, Jan. '75
University of Texas at Austin, Jan. '75.
Tulane University, Jan. '75.
Southwest Research Institute, Jan. '75.
Southern Methodist University, Jan. '75
University of Houston, Jan. '75.
University of Connecticut (Advances in Metallurgy Lecture Series), April '75

He also presented lectures at the ONR Workshop on Plasticity Constitutive Relations (at Texas A & M University, Nov. '74), and at the Gordon Conference on Physical Metallurgy (Rindge, New Hampshire, June '75).

L. Anand presented lectures on "Strengthening Mechanisms in Steels" at the Annual Meeting, AIME, Fall, 1974 and at the Research Laboratory, U. S. Steel Corporation, Spring 1975.

Other Professorial Activities

J. R. Rice served as co-chairman (along with G. R. Leverant, Pratt and Whitney) of the Symposium on Micromechanical Modelling of Deformation and Fracture, sponsored jointly by the ASME Materials Division and the AIME Committee on Mechanical Metallurgy, and held during the June 1975 Summer ASME Meeting at Troy, N.Y. Rice was also co-chairman (along with P. C. Paris, Brown University) of the ASTM Eighth National Symposium on Fracture Mechanics, held at Providence in August 1974.

Personnel Connected with Contract

1. Professorial Staff: J. Gurland and J. R. Rice

2. Technical Assistant: H. Stanton

3. Research Assistants (Graduate Students): L. Anand, J. Chuang*, A. E. Gurson*, K. Kagawa*, R. McMeeking, D. M. Parks, and S. P. Rawal.

*Supported for portion of previous year only.

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