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

Period: July 1975 - June 1976

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Outline of Work in Progress During Period July 1975 - June 1976

1. Localization of plastic flow and inception of ductile rupture
2. Crack tip fracture processes in ductile metals
3. Interfacial strength, including effects of dissolved segregants
4. Particle and sub-boundary strengthening in steels

Summary of Accomplishments and Work in Progress

Major studies have been started on 1) The conditions governing the localization of plastic flow at the onset of rupture. Specific calculations of critical conditions for a number of material models have been made possible through a theoretical framework by which localization is formulated as a constitutive instability, in the form of a bifurcation into a localized mode from a state of previously homogeneous deformation, and 2) The strength of interfaces with and without the presence of dissolved segregants. Criteria for brittle vs. ductile response of an interface were developed on the basis of dislocation mechanisms and thermodynamic relations, and applied to hydrogen embrittlement.

Further progress has been achieved in the analysis of stress and deformation at a crack tip by the application of the large-strain elastic-plastic finite element program developed over the last two years. Work has continued on particle and sub-boundary strengthening in steels and an experimental study of fracture initiation at particles was begun.

1. Localization of Plastic Flow and Inception of Ductile Rupture

a) General framework for localization

It is common to many ductile metals that when deformed sufficiently into the plastic range, a continuously varying deformation pattern gives way to a highly localized mode in the form of a "shear band". Often, the onset of such localized shearing is followed by cavity nucleation and joining in the band, after very little further deformation, so that the onset of localization becomes synonymous with the inception of rupture. Indeed, in many materials the process sets a limit to achievable ductility at a level that is considerably below what could be attained by the more-or-less homogeneous plastic growth to coalescence of the larger voids existing in the material prior to localization. Cases have been cited, e.g., by Cox and Low (Met. Trans., 1974) for 4340 steel, by Hahn and Rosenfield (Met. Trans., 1975) for a series of aluminum alloys, and by Green and Knott (Trans. ASME, 1976) for prestrained free-cutting steels, in which a process of ductile fracture by the growth of voids from large inclusions has been terminated abruptly by shear banding within the ductile ligaments.

The process of localization is of evident importance to the fracture toughness of structural alloys, but the conditions leading to it remain poorly understood. Studies in the last year by Asaro, Needleman, and Rice have explored several approaches to understanding these conditions and their possible relation to plastic flow properties, as well as to microstructural fracture-in-progress events. In Technical Report 43, Rice has reviewed the experimental background for localization and has also presented the theoretical framework by which the condition for localization is formulated as a constitutive instability, in the form of a bifurcation into a localized mode from a state of previously homogeneous deformation. The report includes the specific calculation of critical conditions for a number of material models. These are phrased, in general, in terms of a critical rate of strain hardening, below which localization would be possible even in a body subjected to all-around displacement boundary conditions. The critical hardening rate is, in general, dependent on the nature of the pre-localized deformation field as well as on constitutive parameters; it is particularly sensitive to those parameters which indicate deviations from plastic "normality" or which correspond to "vertex-like" yielding. The former of these is especially destabilizing, as shown by examples in Tech. Rep. 43 for isotropic materials with pressure-sensitive yielding (without corresponding plastic dilation) and for single crystals in which shear stresses other than the Schmid resolved stress enter the criterion for slip on a given system. Both of these models admit possible localizations with a positive rate of strain hardening although, when normality does apply, the hardening rate must be near-zero or negative to permit localization.

In addition, states of deformation for which an instantaneously non-deforming surface exists in the material (e.g., as in plane strain) are found, in general, to be much more inclined to instability than those for

which one does not (e.g., axially symmetric extension or compression). In particular, this is consistent, generally, with the lesser ductility observed in plane strain tension tests than in uniaxial tension, although the differences predicted between the two cases are somewhat reduced when yield vertex effects are included in the constitutive model. /

Needleman has recently initiated studies on the effect of initial imperfections on the onset of localization. These are considered to take the form of small initial non-uniformities of material properties, and the work is being carried out with special reference to cases which would, according to the bifurcation approach, be strongly resistant to localization. Indeed, previous work by Needleman on the analogous problem of local necking in sheet metal forming operations suggests that there can be a pronounced sensitivity to initial imperfections and that these can be as effective as are vertex effects in mitigating the strongly negative hardening rates predicted for localization when simple, isotropic hardening theories are applied to states such as axi-symmetric extension or compression.

In this connection, H. Yamamoto (special graduate student, on leave from Nippon Steel Corp.), working with Needleman and Rice, has recently begun calculations in which a planar layer of material is assumed to exist within a homogeneously deforming outer body, with the layer having properties that make it slightly "weaker" than the outer region. In the circumstances, a homogeneous strain field is induced within the layer, but it differs from the outer homogeneous field. The calculation as presently formulated uses the dilational plastic, constitutive relations developed by Gurson, in Technical Report 39, for void-containing ductile metals. The initial non-uniformity of properties is taken in the form of a somewhat larger void volume fraction within the layer than outside it. The aim of the calculation is to establish conditions at which very large deformations occur within the non-uniform layer, by comparison to deformations in, say, an axially symmetric extension field imposed upon the outer region. The results should show if there is indeed a very strong sensitivity to small non-uniformities of material properties, so that these are the most important determinants of instability under conditions that are far removed from those in which an instantaneously non-deforming surface exists.

(Staff: J. R. Rice, A. Needleman, H. Yamamoto, R. Asaro)

b) Localization in ductile single crystals

It was observed several years ago in studies by Beevers and Honeycombe (Swampscott Fract. Conf., 1959) and Price and Kelly (Acta Met., 1964) on Al alloy single crystals that these exhibit, at a certain stage in their plastic deformation, a concentration of slip into coarse slip zones, and that fracture sometimes results within such a zone shortly after its formation. In Technical Report 43, Rice showed that localizations of this kind can occur, according to the bifurcation analysis, in a crystal undergoing

single slip only when the plastic hardening modulus for the slip system is zero, provided that the criterion for slip is expressible in terms of the Schmid resolved shear stress but is independent of other stress components. Such a non-hardening response can be approached when, e.g., dislocation cutting of precipitates reduces the resistance to shear, and this may in some circumstances provide an adequate basis for localization. But Rice showed also that when non-Schmid stresses enter into the criterion for slip, the material is in a particularly unstable state and localization can then occur with a positive rate of strain hardening.

A specific calculation carried out in Technical Report 43 is that for a crystal slipping in the x_1 direction on planes with normal in the x_2 direction of the x_1, x_2, x_3 cartesian coordinate system, under conditions for which an increment of plastic shear strain is given by

$$d\gamma_{12}^P = \frac{1}{h} (d\sigma_{12} + \mu d\sigma_{13})$$

Here the σ 's are stress components, h is the strain hardening modulus, and the presence of the term multiplied by the dimensionless parameter μ represents the non-Schmid effect. This kind of representation would arise when, e.g., screw segments of dislocations bypass local obstacles by cross slip, in such a way that the increment of shear on the cross-slip plane, as well as that on the primary plane, governs continued primary slip. The formulation is attractive in that the experiments of Price and Kelly suggested an association of the onset of local cross slipping with that of coarse slip banding. Using the above constitutive model, generalized to an elastic-plastic crystal with isotropic elastic moduli, Rice showed that localization will occur when the hardening modulus drops to the value

$$h_{cr} = \frac{1}{4} \mu^2 G$$

when μ is small, where G is the elastic shear modulus. This is a significantly positive critical modulus even when μ is in the range of 0.05 to 0.1 and an effect of this kind may provide a basis for explanation of localizations which set in under rising load.

Continuing work on the problem by Asaro and Rice is directed to two aspects of the problem. First, at the continuum level, a term proportional to $d\sigma_{23}$ has been added on the right side in the expression for $d\gamma_{12}$, so as to represent the effect of the stress component tending to coalesce a screw segment split into partial dislocations, and certain terms that were assumed negligible by comparison to moduli in the original analysis have been included. These have the effect of adding terms of order $\mu\sigma$ to the expression for h_{cr} . Second, a discrete dislocation model of the cross-slip process is being developed for fcc crystals, and from this the parameter μ and another term measuring the effect of the shear stress tending to coalesce the partial dislocations are to be estimated. Cross slip is assumed to occur when the

free energy change ΔG , associated with coalescing and bowing-out a segment of dislocation onto the cross slip plane, vanishes. Expressing ΔG as a function of the prevailing stress components, this gives

$$\mu = (\partial \Delta G / \partial \sigma_{13}) / (\partial \Delta G / \partial \sigma_{12})$$

and our first model calculation finds that $1/\mu$ is approximately twice the number of screw segments which must be piled-up at an obstacle before the cross-slip excursion can be successful. Hence μ becomes larger with increasing ease of cross-slip (fewer dislocations in the queue) and the crystal becomes, according to our analysis, more prone to localization.

(Staff: R. J. Asaro and J. R. Rice)

2. Crack Tip Fracture Processes in Ductile Metals

a) Stress and deformation analysis of large plane-strain opening at a crack tip in a ductile solid

In a study extending over the last two years, the large strain elastic-plastic finite-element program developed by McMeeking and Rice (Int. J. Solids Structures, 1975) has been applied to model the large plane-strain opening of a crack tip in a ductile solid. The results of the analysis are given in Technical Report 44, which is based on a portion of a Ph.D. thesis in preparation by McMeeking. The finite-element approach taken was developed with specific reference to the problem of obtaining numerically accurate results in the near tip region where severe strain gradients exist. Very small elements are thereby required immediately adjacent to the crack tip by comparison to what could reasonably be used to model the far field. Thus a two-step approach has been taken in which an elastic-plastic finite element solution is first developed based on conventional "infinitesimal strain" assumptions, and this solution is employed to set displacement boundary conditions for the large strain analysis on the border of a circular cut-out region surrounding the crack, of radius that is large compared to the distance from the crack tip over which large strain effects are expected to be important.

It is necessary to start the solution with a crack of finite root radius and this is blunted out to approximately five times the initial crack radius as the solution progresses. Further, an interpretation of the results has been found, based on an earlier approach to the problem by Rice and Johnson via plane-strain slip line theory, through which the numerical results for a finite initial crack radius can be used to estimate those corresponding to zero initial radius.

The solution has been carried out for four material models, all under conditions corresponding to contained small scale yielding. Three of the materials have tensile yield strength $\sigma_0 = E/300$ where E is Young's modulus; one of these is non-hardening and the other two exhibit power-law hardening with exponents $N = 0.1$ and 0.2 , respectively. The fourth material is also non-hardening, with $\sigma_0 = E/100$. The Poisson ratio was 0.3 in all cases and the plasticity was treated as Mises isotropic strain hardening in a manner coincident with that proposed earlier by Needleman (J. Mech. Phys. Solids, 1972).

The result of the analysis is a rather detailed prediction, at the continuum elastic-plastic level, of the stress and deformation field prevailing immediately adjacent to the crack tip, in the region within which fracture micromechanisms are normally operative. Hence several features of the results are of direct interest to the interpretation of fracture experiments.

As expected, the results showed that no completely unambiguous definition of a crack tip opening displacement could be given. The results suggest, however, that for the ideally plastic material models the results

based on different "reasonable" measurement points fall in the general range

$$\delta_t \approx 0.55 \text{ to } 0.65 J/\sigma_0$$

where the higher end of the range applies to the higher strength material and the lower end to the lower strength, and where the value of the J Integral is based on a contour lying in the outer elastic region. Also, for the hardening materials, fairly close numerical agreement is found with a simple procedure suggested by Rice (Munich Fracture Conf., 1973), based on an analogy with the anti-plane strain case, in which σ_0 is replaced in the formula for δ_t by the tensile flow stress at an equivalent shear strain of $N/(1+N)$.

The path-dependence of the J Integral, suitably defined for finite deformation, was also studied numerically. It was found that J was essentially path-independent except on contours passing very close to the blunted crack tip; on these the value of J seems to rapidly diminish toward zero as the tip is approached. The results support the current use of the J Integral as a "characterizing parameter" for the outer elastic-plastic field surrounding the crack tip, and hence as a parameter on which the onset of crack growth can be based. However, they also suggest that serious errors are entailed in any applications of the integral which assume path-independence in the region immediately adjacent to the blunting crack tip.

The triaxially elevated stress levels predicted near the blunted crack tip are found to be in remarkably good agreement with the simpler predictions of Rice and Johnson based on slip line calculations. The numerical solution gives, however, a far more accurate estimate of the size scale in the material over which large, triaxially elevated stresses exist. The results have also been presented not only for the plane directly in front of the crack but for those at 22.5° and 45° from it as well.

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

b) Numerical Modelling Techniques for Large Plastic Strain

The assumption of fully plastic material behavior often facilitates the analysis of nonlinear boundary value problems, e.g., crack tip singularities and void growth models, that might otherwise be intractable. Sometimes the results of such analyses are employed in a numerical calculation, as in using analytically obtained near tip stress and displacement fields in a finite element calculation for fully plastic strain intensity parameters. However, fully plastic materials as conventionally modelled are incompressible and the constraint of incompressibility poses significant difficulties in finite element computations (excluding plane stress).

In finite element calculations compressibility is usually dealt with in one of two ways:

1) The simplest procedure is to consider a sequence of problems with increasing effective bulk modulus and then extrapolate to the incompressible limit. This approach is inefficient in that several nonlinear boundary value problems must be solved to obtain one result.

2) The other approach involves the straightforward application of the Lagrange multiplier technique. The introduction of the Lagrange multipliers increases the bandwidth and the order of the stiffness matrix and the solution time of the algebraic equations is proportional to $(\text{bandwidth})^2 \times \text{order}$. Furthermore, the stiffness matrix is no longer positive definite so that numerical stability is not guaranteed. This consideration is particularly important for nonlinear problems where many iterations may be required.

A new approach is being explored which has the potential of eliminating the above mentioned difficulties. In this method groups of simple elements are arranged into "superelements" so that the incompressibility constraints are satisfied within each superelement. These superelements are then used as the building blocks in the finite element grid. The advantages of this approach for the type of problems envisioned here are: (i) most of the work done in imposing the incompressibility constraints can be done once at the beginning of a calculation and need not be repeated at each stage of a nonlinear solution procedure, (ii) the resulting stiffness matrices are positive definite (and symmetric). The bandwidth of these matrices is increased compared with that for the corresponding problem for a compressible material, but the order is reduced, so that the resulting increase in solution time is about 1/4 that for the straightforward Lagrange multiplier approach.

(Staff: A. Needleman)

c) Modelling of crack tip rupture mechanisms

Currently, the solution discussed above is being employed as the basis for analyzing various models of ductile rupture processes in the region adjacent to the crack tip. These include models for void nucleation, growth and coalescence with the crack tip, as well as for void-void interactions and other processes which could lead to a localization of the crack tip deformation field into a shear band emanating from the tip.

Most of the progress made to date is discussed in Technical Report No. 44, where the implications of the finite-element results for fracture criteria based on critical stress, strain, or both are discussed with respect to the transition of fracture mode and the angle of initial crack growth. The report also contains results of void growth calculations within the near tip region, for void sites lying at different initial angles with the crack plane.

The void growth calculations suggest that when voids are easily nucleated and when the initial void sizes, at nucleation, are only very small fractions

of their spacing, coalescence of those voids directly ahead of the crack will occur before it does for those at 45° with the crack line, whereas the opposite becomes true for larger initial void sizes. However, when the void-nucleating particles are more tenacious, as in the spheroidized steels studied by Rawal and Gurland (Int. Conf. Mech. Behav., 1976), the criterion of void nucleation enters the consideration of fracture path as well. Criteria requiring a critical maximum tensile stress for nucleation tend to favor growth straight ahead; those requiring a critical plastic strain favor growth at 45° . In all of this there remains, of course, the possibility of some unstable localization of deformation at the crack tip, brought about either by the rapid nucleation and/or growth of arrays of voids or by some other instability in the plastic flow process. (Attention is called to the section of this report on Localization of Plastic Flow).

A further study of the effect of cementite particles on the fracture toughness of spheroidized carbon steels at low temperatures is based on the results of S. Rawal and J. Gurland (Technical report 41) and is specifically concerned with the size of the highly stressed region at the crack tip in which unstable cleavage fracture is nucleated and propagated. Ritchie, Knott and Rice (RKR) stipulate a region of 1-2 grains in which a critical cleavage stress is achieved. By matching the experimental K_{IC} values of our steels with the RKR procedure, we obtain an average size of 1.3 grains. Our results support the RKR model for cleavage fracture and suggest that the critical event includes the propagation of the crack through a grain boundary, thereby requiring the highly stressed region to be larger than one grain. Good agreement was obtained between measured K_{IC} values and those calculated by the RKR procedure not only under linear elastic stress conditions but also for small scale yielding conditions (with plastic-elastic stress distribution) provided that the mode of fracture initiation is by cleavage, as, for example, in steels of high carbon content and at low testing temperatures.

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

d) Crack formation at particles

An experimental program has been started to study crack formation at inclusions and particles during the early stages of fracture. The current work attempts to elucidate the conditions of crack initiation at Fe_3C particles by interfacial separation or particle cracking in steels. The controlled variables are 1) the composition of the steels, namely carbon content in the range 0.1 to 1.05% C, 2) the state of stress, i.e. uniaxial in smooth specimens or triaxial in notched geometries, and 3) the temperature, in the range -196° to $20^\circ C$. The techniques of microscopic observation include optical microscopy of sections through the deformed specimen, scanning electron microscopy of fracture surfaces, and, eventually, transmission electron microscopy of thin sections. Interesting preliminary results are that particle fracture is a much more common occurrence than interfacial separation when the particles are dispersed, but that interfacial void formation is often associated with the matrix film between clustered particles.

(Staff: J. Gurland and J. Fisher)

3. Interfacial Strength (Including Effects of Dissolved Segregants)

a) Criterion for brittle versus ductile response of an interface

A study has been initiated this year on determining those factors which make possible the brittle versus ductile response of an interface to a stress concentration, with particular reference to the role of a dissolved segregant, particularly hydrogen, in affecting this response. The motivation for focusing on interfaces, e.g., between grains or phases or between particles and the surrounding matrix, is that these are often observed, fractographically, to provide the path of a brittle fracture, or to provide the brittle nucleation portion of what is, ultimately, a ductile fracture by growth to coalescence of cavities nucleated at particles or inclusions. Interfaces seem no less pervasive as fracture paths in H embrittled metals, but most previous work on the problem has been directed instead to H effects on the cleavage of a crystal lattice. This case can be recovered by specialization to the case of an interface between identical phases, but it seems to be of more general applicability to address the problem of H and like segregant embrittlement effects in terms of the effect on the strength of an interface.

In work reported as Technical Report No. 40, Rice has derived a condition for stability against dislocation nucleation of an atomistically sharp interfacial crack, when its tip region is stressed to the critical Griffith condition appropriate to the interface. If a positive energy barrier exists against nucleating a dislocation from the tip at this condition, it is assumed that the interface can exhibit atomistically brittle cleavage, and the only requirement is that sufficient local stress be exerted on the interface to nucleate and spread such a crack. If, instead, there is no energy barrier, any such crack tip is unstable in the sense that it will blunt out in response to the stress concentration through dislocation nucleation. The calculation follows along similar lines to that of Rice and Thomson (Phil. Mag., 1974) for lattice cleavage, and is similarly approximate in that core cut-off parameters are introduced and crystal elastic anisotropy is neglected. The results, from Technical Report No. 40, can be summarized as follows: If $(r_0/b)(\gamma_{int}/\gamma_{lat})$ is less than approximately 2/3 (the exact value depends on the orientation of the slip plane and slip direction relative to the interface) there is a positive energy barrier against dislocation nucleation and the interface can sustain an atomistically sharp cleavage crack. Here b is the Burgers vector and r_0 the core cut-off radius for the dislocation being tested; γ_{lat} is the surface energy of the step left at the crack tip by emission of a dislocation and γ_{int} is defined so that $2\gamma_{int}$ is the work of reversible separation of the interface. On the other hand, if $(r_0/b)(\gamma_{int}/\gamma_{lat})$ is greater than approximately 2/3, the interface can sustain an atomistically sharp crack only if $\gamma_{lat}/\mu b$ is sufficiently small, where μ is the shear modulus. For example, if $(r_0/b)(\gamma_{int}/\gamma_{lat}) = 1$ the sharp crack can be sustained only if $\gamma_{lat}/\mu b$ is less than approximately 0.8 where, again, the exact value is orientation dependent.

The calculation could be refined to more fully reflect crystalline anisotropy and, in this connection, Asaro has recently obtained the solution for the force

arising from image effects on a near-tip dislocation in a cracked crystal of arbitrary elastic constants. This should provide a useful first step toward understanding the role of elastic anisotropy in determining brittle versus ductile response. Also, current work by Mason, a Research Assistant on the project, is aimed at assessing the effect of orientation of the crystals which adjoin at the interface on the issue of brittle versus ductile response. As noted above, the predicted critical conditions are orientation dependent and her work is directed toward developing a computational search for the range of orientations, if any exist at all, which allow brittle grain boundary separations in a polycrystal.

This analysis is being carried out with particular reference to Cu polycrystals containing small concentrations of bismuth segregated at grain boundaries, since the concentrations required for embrittlement and the corresponding alterations of cohesive energy are fairly well documented experimentally for this case in recent work by Hondros and McLean (Phil. Mag., 1974). An earlier application of the theory to H embrittlement of fcc polycrystals by Rice (Tech. Rep. 40) suggested that within uncertainties stemming from orientation dependence and other factors, the observed embrittlement of normally ductile Ni polycrystals by dissolved hydrogen is consistent with energy lowerings that are estimated from Gibbs adsorption isotherms for H on Ni surfaces. In particular for a choice of core size parameter between b and $2b$ for the fcc lattice, the surface energy lowering required to embrittle a Ni grain boundary is estimated to lie between approximately 0.18 to 0.75 J/m²; this range seems to be well within what can be achieved, e.g., by electrolytic charging.

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

b) Thermodynamic relations governing cohesion in presence of a mobile segregant

As a further aspect of Tech. Rep. 40, Rice showed that by considering the stress on a segregant-containing interface, or the partial separation across it, as another state variable for the interface, it is possible to derive relations between basic cohesive properties and the variation of interface adsorption with separation. In particular, the Gibbs relation at isothermal conditions (and, for simplicity, with constant strain in the plane of the interface) is

$$\sigma d\delta + \mu d\Gamma = d\phi$$

where ϕ is the surface free energy, Γ the surface segregant concentration, μ the equilibrating segregant potential, δ the excess opening displacement across the interface, and σ the normal stress. There follows the relation

$$(\partial\sigma/\partial\mu)_{\delta} = -(\partial\Gamma/\partial\delta)_{\mu} \quad ,$$

and from it relations for the change with μ of the work of separation at constant μ and the cohesive strength at constant μ have been obtained. For example, if $2\gamma(\mu)$ is defined as the work of separation at constant μ , then

$$2d\gamma(\mu)/d\mu = - [\Gamma_{\infty}(\mu) - \Gamma_0(\mu)] \quad ,$$

when $\Gamma = \Gamma_0(\mu)$ and $\Gamma = \Gamma_{\infty}(\mu)$ are the respective adsorption isotherms for the unstressed interface and for the completely separated surfaces. This result is a generalization of the Gibbs adsorption theorem to interfaces.

Separation at constant μ corresponds to very slow, quasi-equilibrium separation and can be approached experimentally only when the segregant is mobile, e.g. as for H in the bcc Fe lattice at room temperature. The opposite extreme is separation at constant segregant, and analogous expressions were derived which relate the work of separation and cohesive strength at constant Γ to variations of adsorption behavior with separation.

It was shown also that even though, in principle, the presence of a segregant can either weaken or strengthen an interface, the work of separation at constant μ can never exceed that at constant Γ . This points to an important role of solute mobility which may be central to many embrittling effects observed with H. In particular, a given solute may weaken an interface merely by its presence there, but an additional embrittlement arises when the solute is mobile so that conditions for separation at constant μ can be approached. It is possible that the kinetics of local H transport to fracture sites, induced so as to more nearly achieve conditions of constant μ , and hence those of maximum embrittlement, is central to setting the time dependence observed in H embrittlement phenomena, and this is the subject of continuing work.

(Staff: J. R. Rice)

c) Elevated temperature diffusive rupture

Work was continued on the examination of various nonequilibrium aspects of the elevated-temperature diffusive growth of creep rupture cavities on grain boundaries. This is thought to be an important mechanism at temperature ranges of approximately 0.5 to 0.8 T_m , but at low stress, long lifetime conditions for which dislocation effects are minimal. The classical Hull-Rimmer model of the diffusive rupture process, by matter transport from the cavity walls into the adjacent grain boundary, assumes a quasi-equilibrium cavity shape (spherical, for an isotropic material) whereas a model introduced recently by Chuang and Rice deals with the opposite limiting case in which surface diffusion is sufficiently slow that the rupture cavity is long and crack-like. Both models allow a simple solution for the relation of the applied stress to cavity growth rate, based on the assumption that the adjoining grains separate as rigid bodies so as to

accommodate matter which is diffused from the cavity walls into the grain boundary; but there has been no criterion available to decide which model is more nearly appropriate in given circumstances.

The problem has been addressed in the Sc.M. thesis by Kagawa, reprinted as Technical Report 42. In this, a simple self-similar solution of the linearized surface diffusion equation is derived which may be made to give results coincident with either of the two limiting cases by appropriate choice of a parameter measuring the cavity expansion rate. In particular, in the self-similar solution all cavity dimensions increase in proportion to $t^{1/4}$ where t is time and the cavity grows from vanishing small size at $t = 0$. Writing the cavity length as $a = \beta t^{1/4}$, it is found that the resulting shape is spherical as in the Hull-Rimmer model when β is small, whereas the shape for large β approaches, near the cavity tip, that of the Chuang-Rice crack-like model. By plotting predictions of the self-similar model together with the two models in which the cavity shape is assumed a priori, Kagawa suggests that to a reasonable approximation the Hull-Rimmer model may be adopted when $a^3 da/dt$ is less than a certain value, and the Chuang-Rice model when it is greater, where the transition value depends on material and temperature-dependent transport properties.

Tech. Rep. 42 also contains an extensive catalog of expressions for diffusive relaxation times, with numerical values given for several metals at $0.5 T_m$ and $0.8 T_m$. These relaxation times are defined for a sinusoidal disturbance in the shape of a free surface, and also for a sinusoidal normal misfit displacement along an interface between two elastic crystals. The processes considered include, for the free surface relaxation times, surface self-diffusion, lattice self-diffusion, and evaporation-condensation. For the misfitting interface they include grain-boundary and lattice self diffusion. While there are considerable variations between materials, and also in surface diffusion coefficients as taken from different literature sources for the same material, it appears that the processes of shortest relaxation times, for disturbances of wavelength on the order of $10\mu m$ or less, are provided by surface and grain-boundary self-diffusion in general.

(Staff: J. R. Rice and K. I. Kagawa)

4. Particle and Sub-Boundary Strengthening in Steels

As part of a comprehensive program on the deformation and fracture properties of carbon steels, L. Anand and J. Gurland studied the strain hardening behavior of a variety of spheroidized steels. The main objective of this study was a determination of the individual contribution to the overall strain hardening behavior arising from grain boundaries, subgrain boundaries and cementite particles. One important contribution to both strain hardening behavior and fracture initiation is the development of rather large internal stresses at the particle matrix interfaces caused by the incompatibility in plastic strains between the ductile matrix and undeformable particles. Recent theoretical developments by L. M. Brown and W. Stobbs (Phil. Mag. 1971) and R. J. Asaro (Acta Met. 1975) have made direct links between these internal stresses and the dislocation substructures that develop in the vicinity of the particles. Furthermore these internal stresses and dislocation substructures can be quantified experimentally through measurements of Bauschinger effects as shown again by Brown and separately by Asaro. This past year Y. W. Chang has begun cyclic deformation studies on 1.4% and .8% carbon steels to measure those Bauschinger effects and internal stresses and to quantitatively determine their contribution to strain hardening. Special grips suitable for such testing have been designed and built. Heat treatments that produce the desired particle and sub-boundary structures in these steels have also been developed by Chang. We plan to do the mechanical testing presently, and expect to conclude our study by this summer. Our measurements should complement those of Anand and Gurland in an important way especially with regards to the proposed fracture studies of J. Fisher and J. Gurland on similar alloys.

In connection with this experimental study, some effort was devoted to refine the strain hardening model of particle reinforced alloys as described by L. Anand and J. Gurland in last year's progress report (Technical Report 100-3084-37). Two specific problems were examined further, namely the superposition of the effects of statistical and geometrically necessary dislocation densities, and the effect of the unrelaxed back stress due to dislocation tangles around hard particles. These points were incorporated into the publication based on the technical report (L. Anand and J. Gurland, Acta Metallurgica, to be published).

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

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- COO-3084-40 J. R. Rice, Hydrogen and Interfacial Cohesion, October 1975.
- COO-3084-41 S. P. Rawal and J. Gurland, Observations on the Effect of Cementite Particles on the Fracture Toughness of Spheroidized Carbon Steels, February 1976.
- COO-3084-42 K. I. Kagawa, Models of Slow Intergranular Void Growth Due to Void Surface and Grain Boundary Self-Diffusion, February 1976.
- COO-3084-43 J. Rice, The Localization of Plastic Deformation, April 1976.
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- L. Anand and J. Gurland, Effect of Internal Boundaries on the Yield Strength of Spheroidized Steels, Metallurgical Transactions (1976) 7A, p. 191-197.
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- *D. M. Parks, Interpretation of Irradiation Effects on the Fracture Toughness of a Pressure Vessel Steel in Terms of Crack Tip Stress Analysis; Transactions ASME, Journ. of Engin. Materials and Tech., Vol. 98, 1976, p. 30-36.
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J. R. Rice, Hydrogen and Interfacial Cohesion; in Effects of Hydrogen on Behavior of Materials (eds. A. W. Thompson and I. M. Bernstein), Metallurgical Society of AIME, 1976, p. 455-466.

J. R. Rice, The Localization of Plastic Deformation; in Proceedings of the 14th International Congress of Theoretical and Applied Mechanics (Delft, 1976), Vol. 1, North-Holland Publishing Co., In Press.

*J. R. Rice, Continuum Mechanics and Thermodynamics of Plasticity in Relation to Microscale Deformation Mechanisms; in Constitutive Equations in Plasticity (ed. A. S. Argon), M.I.T. Press, 1975, p. 23-79.

* Previously listed as "in press."

Thesis

K. I. Kagawa, Sc.M. Thesis, "Models of Slow Intergranular Void Growth Due to Void Surface and Grain Boundary Self-Diffusion," February 1976.

Oral Presentations

J. R. Rice presented seminar talks on the work relating to interfacial cohesion and hydrogen embrittlement effects at Brown (Nov. '75) and at Princeton University (Nov. '75). He also spoke on this topic as a member of the Panel Discussion group at the AIME Meeting on Hydrogen Effects on Behavior of Materials (September 1975). He also gave an invited lecture on "Computational Continuum Mechanics with Application to the Plasticity and Fracture of Solids" at the Conference on Computer Simulation for Materials Applications, NBS, April 1976.

R. M. McMeeking presented seminar talks on the finite-element analysis of large deformation effects in crack tip opening at Princeton University (January 1976), General Electric Corp. (May 1976), and the University of Illinois (May 1976).

R. Asaro presented seminar talks on "Localized Plastic Deformation in Single Crystals," at Stanford University, (February 1976) and Massachusetts Institute of Technology, (March 1976) and "Localized Plastic Deformation in Metals," at Harvard University, (April 1976). He also presented a lecture on "Applications of the Geometric Theorems for Dislocations in Anisotropic Elastic Media," at the Conference on Computer Simulation in Materials Science, NBS, Gaithersburg, Maryland, (April 1976).

Personnel Connected with Contract

1. Professional Staff: R. J. Asaro, J. Gurland, A. Needleman and J. R. Rice
2. Research Engineer: L. Hermann
3. Technical Assistant: H. Stanton
4. Research Assistants (Graduate Students): Y. W. Chang, A. L. Gurson*, J. R. Fisher, D. Mason*, R. M. McMeeking, K. I. Kagawa* and H. Yamamoto**.

* Supported for portion only of contract period.

** Not supported by contract.

Present Position of 1975 Graduates Connected with Contract

- L. Anand, Ph.D., 1975, Research Engineer, Research Laboratory, U.S. Steel Corp., Monroeville, Pennsylvania.
- T. J. Chuang, Ph.D., 1975, Mechanical Engineer, Engineering Services, Westinghouse Electric Corp., Pittsburgh, Pennsylvania.
- A. E. Gurson, Ph.D., 1975, Mechanical Engineer, Systems Division, Avco Corp., Wilmington, Massachusetts.
- D. M. Parks, Ph.D., 1975, Assistant Professor, Department of Engineering and Applied Science, Yale University, New Haven, Connecticut.
- S. P. Rawal, Ph.D., 1975, Research Engineer, N.E. Metals Co., Manville, Rhode Island.