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# Dynamic-Viscoplastic Experiments and Analyses of Rapid Crack Propagation and Arrest

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# ABSTRACT

There are many practical situations in which the initiation of rapid crack propagation cannot be absolutely precluded and where the consequences of a large scale fracture would be catastrophic. For these cases crack arrest The currently available fracture mechanics technology is needed. procedures utilize elastodynamic analyses and material fracture property characterization. However, as small-scale yielding conditions are not always satisfied, more advanced viscoplastic-dynamic analyses are now being developed to generalize the technology. The approach that has been taken in the SwRI work is to intimately couple a viscoplastic-dynamic analysis capability with exceptionally-well instrumented fracture propagation experiments. This level of complexity is deemed essential to ensure transferability of arrest toughness values obtained from small size test specimens to an engineering structure when inertia forces, reflected stress waves, large-scale yielding and the rate-dependence of yielding must be accounted for. Following a pragmatic introduction to the subject, this paper outlines the current technology and suggests the areas in which further research is needed.

# KEYWORDS

Crack arrest; dynamic fracture mechanics; viscoplasticity; coupled pressure bar experiment; nuclear pressure vessels; A533B steel; storage tanks.

#### INTRODUCTION

From the time of A. A. Griffith through the first of these International Conferences on Fracture, the subject of fracture mechanics was largely of academic interest only. It is only over the past two decades that the technology has become of widespread practical usefulness. One factor is responsible: given the significant advances that have been made both in flaw detection and in the capability to perform accurate structural analyses, fracture mechanics is uniquely able to balance assurance for safe operation against the costs of materials, inspection and maintenance.

Fracture mechanics technology, at first limited to consideration of crack instability, became of wide interest in practical engineering only when its uses were expanded to quantify crack growth. This advancement occurred first for subcritical crack growth by fatigue and creep. Despite an earlier beginning, the quantification of crack growth at the opposite end of the time spectrum occurred later. Indeed, the branch of fracture mechanics dealing with rapid crack growth, generally called "dynamic fracture mechanics," is only now coming to maturity.

This paper will touch on both theory and applications in the belief that the most effective research is that in which the two directly interplay. To highlight this coupling, in this paper the term dynamic fracture mechanics will be used only when the basic technology is the focal point. The term "crack arrest fracture mechanics" will be used when applications to engineering structures are the prime concern.

Two pragmatic concerns were largely responsible for the establishment of dynamic fracture mechanics. Concern for "brittle" fracture in ship hulls led the Navy Research Laboratory to take a pioneering role in the subject, and, subsequently, led the Office of Naval Research to support a body of basic theoretical work. Independently, the Nuclear Regulatory Commission and the Electric Power Research Institute supported combined experimental and computational work to investigate the potential for crack propagation in a nuclear power plant pressure vessel. While not all aspects of the subject are completely understood, the totality of the progress achieved in these separately supported research efforts permits a good number of engineering applications of crack arrest fracture mechanics to be made. Ironically, it may be that other application areas - e.g., gas transmission pipelines and storage tanks - may ultimately be a greater beneficiary of this progress than the two application areas that spawned it!

This paper contains three major sections. First, the need for crack arrest fracture mechanics is illustrated by consideration of a recent field failure. Second, the principles underlying current applications of the technology are elucidated. Third, progress in the development of practical techniques for the determination of the arrest toughness of ductile and tough materials via viscoplastic-dynamic analyses and experiments is presented. The objective of the paper is to provide an assessment of current progress and, in so doing, to identify the critical unresolved issues that will provide a point of departure for future research.

### THE NEED FOR CRACK ARREST FRACTURE MECHANICS

A particularly illustrative example of the need for procedures to ensure crack arrest is one in which this technology was evidently not utilized. This example is the re-built oil storage tank that failed near Pittsburgh, Pa., on 2 January 1988. This accident caused about one million gallons of oil to spill into a nearby river, thereby contaminating the water supply of a large number of municipalities in Pennsylvania, West Virginia and Ohio. Specifically, a 120 feet diameter tank was filled to nearly its full height of 48 feet when it failed by the initiation of a brittle cleavage crack that propagated vertically to split the tank (Mesloh et al., 1988; Gross et al., 1988). The crack emanated from a "dime-sized" flaw below a horizontal weld joining the first and second courses of steel plates at a point about 8 feet above the base of the tank.

The flaw had a dimension of 0.74 inches (about two thirds of the wall thickness) and was located in the base metal. As a result of the embrittlement caused by cutting and by subsequent welding adjacent to the flaw, the base metal adjacent to the flaw was substantially less tough than that of normal base metal (Mesloh  $\underline{\text{et}}$  al., 1988). In addition, while the stress at the initiation site due to the contained oil was only about 12 ksi, tensile residual stresses apparently acted to increase the actual stress to about 30 ksi. Thus, the stress in the region of the flaw at the instant of the failure was reported to have been about 85% of the yield stress. All in all, it is not therefore surprising that rapid crack propagation was initiated in this instance.

It cannot be assumed that the conditions that existed in this incident are unique. The existence of imperfect weldments or similar types of abnormal regions that can trigger a rapidly propagating crack cannot be precluded in any type of structure. Similarly, there are a considerable number of engineering structures that are vulnerable to third-party damage and other unforeseeable events wherein fracture instability leading to the initiation of rapid fracture cannot be absolutely precluded; e.g., a gas transmission pipeline. Here also, structural integrity can be assured if crack arrest occurs to prevent a catastrophic rupture. More specifically, the basis of crack arrest fracture mechanics is to assure that the sound material that is encountered by the crack as it exits a defected or damaged region will arrest the crack.

Implicit in the crack arrest fracture mechanics point of view applied to a pressure boundary, if crack arrest occurs to prevent a catastrophic fracture, the leaking of the contained fluid should trigger operator intervention to preclude further danger. However, there is a possible fallacy in this approach in that it ignores the size of the leak. For example, one of the largest industrial accidents of all time--the LPG storage tank rupture near Mexico City on 19 November 1984--apparently resulted from a leak that ignited and exploded (Pietersen et al., 1985). This caused a fragmenting type of rapid fracture event that greatly magnified the consequences of the disaster to include 500 fatalities, 7000 injuries, and uncountable other damage.

The foregoing should amply demonstrate the need to avoid the enormous consequences of a catastrophic accident. At the same time, it should also be clear that excessive conservatism in the name of safety can not only be costly, in some instances conservatism can actually be counterproductive; e.g., from improperly performed weld repairs. The requirements for safety during operation must always conflict with the need for economy in design, construction and maintenance. This inevitable conflict clearly points to the need for accurate structural integrity assessments that is afforded only through the proper application of fracture mechanics.

# ELASTODYNAMIC FRACTURE MECHANICS

A key element of crack arrest fracture mechanics is the crack arrest toughness property of the component material. The controversy between the static and dynamic views of this parameter has been largely resolved through the general acceptance of the idea that the crack arrest toughness is connected to the propagating fracture resistance. This follows from the notion that rapid crack propagation is governed by an equality between the dynamically computed crack driving force and the material's resistance to crack extension. For small-scale yielding conditions, this can be expressed as

$$K (a,\sigma,t) = K_D(V,T)$$
 (1)

where  $K_{\rm D}$ , the dynamic (or running) fracture toughness, is a thickness-dependent material property that depends on the crack speed V and the ambient temperature T, while K is the dynamically calculated value of the stress intensity factor; a function of crack length a, applied stress  $\sigma,$  and time t. Crack arrest occurs when K becomes less than the minimum value of  $K_{\rm D},$  and remains less for some long period of time.

Equation (1), which is valid for small-scale yielding conditions, follows from the "crack tip dominance" argument that is the basis of modern fracture mechanics - see Kanninen and Popelar (1985). The central idea of this argument is that the inelastically deformed material that inevitably attends the crack tip need not be explicitly considered provided it is contained within a region that is dominated by the singular term in the crack tip stress field. When this is so, if in addition the bulk of the material is essentially linear elastic, then the term

$$\sigma_{ij} = \frac{K}{(\pi r)^{\frac{1}{2}}} F_{ij}(\theta, V)$$
 (2)

will dominate. Here,  $\theta$  and r denote polar coordinates located at the tip of a crack that is propagating with an instantaneous speed V, and F is a universal function of order unity. Because the applied stresses, component dimensions and crack length affect the local deformation field only through K - to the extent that the local heat generation and the wake of inelastically deformed material that trails the crack tip can be ignored - Equation (1) follows.

While detailed studies such as those of Hudak et al (1986) have given disquieting exceptions, the acceptable  $\rm K_D$  values that have been obtained generally have a common form. As a function of crack speed and temperature, these data can often be correlated by the heuristic relation

$$K_{D} = \frac{K_{A}}{1 - (\frac{V}{V_{C}})^{m}}$$
(3)

where  $K_{\mbox{\scriptsize A}}$ ,  $V_{\mbox{\scriptsize C}}$  and m are empirical temperature-dependent material constants. Because  $K_{\mbox{\scriptsize A}}=K_{\mbox{\scriptsize A}}(T)$  is the minimum value of  $K_{\mbox{\scriptsize D}},$  it represents the dynamic crack arrest toughness of the material.

It is noteworthy that the parameter  $\rm V_{\rm C}$  is generally much less than the elastic wave speeds whereupon the observed crack speeds are confined to a fraction of these values. However, of more significance for characterizing crack arrest, results of the type that can be represented by Equation (3) indicate that static interpretations of crack arrest toughness obtained under the proper conditions will be identical to  $\rm K_{\rm A}$ . In particular, this will be the case if arrest occurs before stress waves are reflected back to the crack tip from the specinen boundaries. Although it has yet to be conclusively demonstrated, Equation (3) also suggests the possibility that valid  $\rm K_{\rm A}$  data can be obtained where crack arrest does not occur; i.e., by extrapolating the  $\rm K_{\rm D}$  data base to zero crack speed.

A procedure that has been found to be effective for generating  $K_{\overline{D}}$  data is a hybrid experimental/computational procedure known as a "generation-mode" analysis. In this procedure, experimental crack length and load point displacement, both as functions of time, are taken as input to a computational simulation of the experiment. These data specifically allow an initial value, moving boundary value problem to be solved. The solution, in turn, determines the dynamic stress intensity factor history. By invoking Equation (1),  $K_{\overline{D}}$  values for the material as a function of crack speed and temperature can then be inferred.

The counterpart of a generation-mode analysis is an "application-mode" analysis. This requires  $K_{\text{D}}$  data to be available at the outset; e.g., in the form represented by Equation (3). Then, for specified initial and boundary conditions, a prediction of crack length versus time (including crack arrest, if it occurs) can be obtained. Figure 1 illustrates these procedures as they have been used at SwRI for the goal of assuring nuclear pressure vessel integrity through crack arrest, Dexter et al (1987).

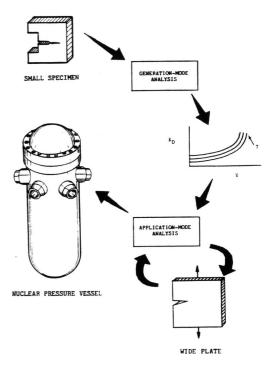


Fig. 1. Illustration of the experimental/computational coupling used to determine and verify fracture toughness data from small-scale tests for application to a nuclear pressure vessel.

Figure 2 shows a comparison of an elastodynamic application-mode calculation for a wide plate test conducted at the U.S. Bureau of Standards (NBS) for the Nuclear Regulatory Commission's Heavy Section Steel Technology (HSST) Program - see deWit et al (1988). In this series of tests, one-meter wide plates of nuclear pressure vessel A533B steel were subjected to a temperature gradient such that crack propagation, initiated at a low temperature, would be arrested at a higher temperature. The computational result shown in Figure 2 compares an application-mode elastodynamic calculation of crack length versus time with NBS timing wire data. The computation was based upon a simplified version of Equation (3) given by (metric units)

$$K_{ID} = K_{IA} + A V^2$$

where

$$K_{TA} = 49.957 + 16.878 \exp \left[.028738(T-RT_{NDT})\right]$$

and

$$A = \begin{cases} [329.7 + 16.25 (T-RT_{NDT})] \times 10^{-6} & T \ge 13.9 \text{ °C} \\ [121.71 + 1.296 (T-RT_{NDT})] \times 10^{-6} & T \le 13.9 \text{ °C} \end{cases}$$

in which  $RT_{\rm NDT}$  is a reference temperature related to the transition temperature. For the A533B steel used in the HSST program,  $RT_{\rm NDT}$  = -23°C.

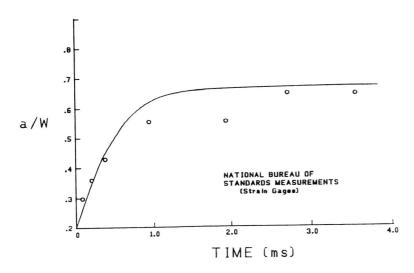


Fig. 2. Comparison of an elastodynamic application mode computation and experimental data for a wide plate test on A533B steel conducted by the National Bureau of Standards.

# VISCOPLASTIC-DYNAMIC FRACTURE MECHANICS

The methodology outlined in the above will be appropriate provided that small-scale yielding conditions are valid. When this is not the case—either in the material fracture property characterization experiments and/or in the application itself—then it is necessary to directly confront the inelastic behavior. However, for a rapidly moving crack, the material directly ahead of the crack tip is subjected to enormous strain rates. It is therefore apparent that a treatment that is concerned with large real plastic deformation must include the rate dependence of yielding. This mandates a viscoplastic-dynamic approach. Implementing such an approach requires both appropriate material constitutive behavior to be instituted and a near—tip dominating parameter to be quantified, in addition to well—instrumented companion experiments from which appropriate material property data can be extracted.

# Viscoplastic Material Behavior

While a variety of viscoplastic representations are possible, work at SwRI has taken the approach developed by Bodner and Partom. The relations are summarized as follows. First, the flow law is expressed as:

$$\stackrel{\bullet}{\epsilon}_{ij} = \stackrel{\bullet}{\epsilon}_{ij}^{e} + \stackrel{\bullet}{\epsilon}_{ij}^{p} \tag{4}$$

$$\stackrel{\bullet}{\epsilon}_{ij}^{p} = \lambda S_{ij}; \quad \stackrel{\bullet}{\epsilon}_{kk}^{p} = 0$$
(5)

with 
$$S_{ij} = \sigma_{i,j} - \frac{1}{3} \delta_{i,j} \sigma_{kk}$$
 (6)

Next, the kinetic equations are:

$$D_2^p = D_0^2 \exp \left[ -\left(\frac{Z^2}{3J_2}\right)^n \right] \tag{7}$$

with 
$$Z = Z^{I}$$
 (8)

$$D_2^{p} = \underset{\varepsilon}{\mathbf{i}} \underset{\varepsilon}{\bullet} \underset{i}{\bullet} \underset{\varepsilon}{\bullet} p$$
 (9)

$$J_2 = {}^{1}_{2}S_{ij}S_{ij} \tag{10}$$

$$\lambda^2 = 0_2^p / J_2 \tag{11}$$

The evolution equation of isotropic hardening internal variables is given by:

$$\tilde{Z}^{I} = m_{1} (Z_{1} - Z^{I}) \hat{w}_{p}$$
 (12)

with 
$$Z^{I}(o) = Z_{o}; \quad \overset{\bullet}{w_{p}} = \sigma_{i,j} \varepsilon_{i,j}^{p}; \quad w_{p}(o) = 0$$
 (13)

The material constants  $D_{\rm O}$ ,  $Z_{\rm O}$ ,  $Z_{\rm I}$ ,  $m_{\rm I}$ , n must be determined empirically. These constants have been developed at SwRI for nuclear pressure vessel steel, a cryogenic storage tank steel, and a line pipe steel. As an illustration, Fig. 3 compares the experimentally measured stresses at 10% plastic strain and the stresses predicted by this model at several temperatures for A533B steel. This typifies the good agreement that is generally obtained.

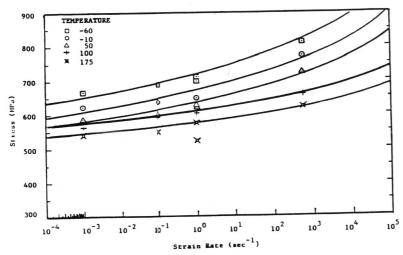


Fig. 3. Comparison of the experimentally determined stress at 10 percent plastic strain with the Bodner-Partom model for A533B steel as a function of strain rate and temperature.

It should be recognized that a number of viscoplastic formulations exist that provide alternatives to the use of Equations (4-13); e.g., that of Perzyna (1966). As each of these alternatives contains disposable parameters, they will all generally be adequate in the strain rate range in which tests can routinely be conducted; i.e.,  $\dot{\epsilon} < 10^4~{\rm sec}^{-1}$ . Accordingly, the most appropriate formulation is one that can be used to extrapolate the data into the very high strain rate region, perhaps  $10^8~{\rm sec}^{-1}$ , that may be experienced at the tip of a fast propagating crack. Unfortunately, no combination of theory and experiment yet exists to distinguish between the various approaches. This is one of several key issues that future research in this subject most resolve.

# Characterizing Parameters for Viscoplastic-Dynamic Fracture Propagation

Just as for the elastodynamic approach, in materials exhibiting viscoplastic behavior, the asymptotic fields in the neighborhood of the crack have an important bearing on the crack tip characterizing parameter. Recent work in this area has focused on examining the strength of the singularity for a rapidly propagating crack in a material whose

response is governed by the Bodner-Partom law; Achenbach et al (1985), Freund (1987), Popelar (1987) and Sheu (1988). Their research has shown that an elastic singularity exists near the crack tip since the elastic strain rates dominate the plastic strain rates. However, for materials of practical interest, this region is extremely small with some estimates being 1/1000 of the plastic zone in a small scale yielding situation. The usefulness of this elastic crack tip singularity and its attendant crack tip stress intensity factor is unresolved for practical applications.

While a geometric criterion known as a crack tip opening angle (CTOA) has shown some promise, most of the several parameters that have been proposed as fracture criteria are based on crack tip integrals; e.g., a dynamically-enhanced J-integral. However, it can be shown that most of the crack tip integrals are merely specializations of a general class of integrals that was introduced by Atluri (1982). The G parameter developed by Moran and Shih (1987) is essentially identical to this integral.

The incremental form of Atluri's relation is given by:

$$\Delta T^* = \lim_{r \to 0} \int_{r} [(\Delta W + \Delta P)n_1 - (\sigma_{ij} + \Delta \sigma_{ij})n_j \Delta u_{i,1} - \Delta \sigma_{ij}n_j u_{i,1}] dr$$
 (14)

where W is the stress work density and P is the kinetic energy density. The quantities  $n_i$  are the components of the vector normal to the contour shown in Fig. 4. It is assumed in Fig. 4 that the crack is propagating in the  $\mathbf{x}_1$  direction. The parameter  $\mathbf{T}^*$  is computed from equation (14) through a simple summation

$$T^* = \sum_{i=1}^{n} (\Delta T^*)_i$$
 (15)

where n denotes the current number of time increments.

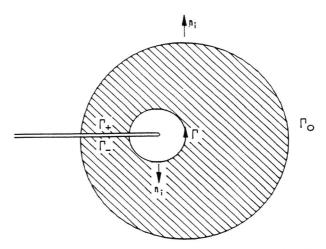


Fig. 4. Integral path definition in the vicinity of the crack.

A critically important aspect of equation (14) is that its value is independent of the contour only in the limit as the inner contour shrinks onto the crack tip. Consequently, unlike the J-integral for deformation plasticity and quasi-static crack growth, the T parameter is path independent only in a local sense.

From a computational point of view, equation (14) does not permit a suitable means for calculating the integral. However, application of the divergence theorem transforms the integral into a more convenient far field contour and a volume term. This results in

$$\Delta T^{*} = \int_{\Gamma_{0}} [(\Delta W + \Delta P)n_{1} - (\sigma_{ij} + \Delta \sigma_{ij})n_{j}\Delta u_{i,1} - \Delta \sigma_{ij}n_{j}u_{i,1}]d\Gamma$$

$$+ \rho(u_{i} + \Delta u_{i})\Delta u_{i,1} - \rho(u_{i} + \Delta u_{i})\Delta u_{i,1} + \rho\Delta u_{i}u_{i,1} - \rho\Delta u_{i}u_{i,1}]dA \qquad (16)$$

$$+ \int_{\Lambda_{0}} [\Delta \sigma_{ij}(\varepsilon_{ij,1} + 1/2 \Delta \varepsilon_{ij,1}) - \Delta \varepsilon_{ij}(\sigma_{ij,1} + 1/2 \Delta \sigma_{ij,1})$$

The connection between the J integral and the stress intensity factor has been well documented for materials where the HRR singularity exists, Kanninen and Popelar (1985). A more complicated situation exists for a growing crack in a rate dependent inelastic material since the relationship of the singularity at the crack tip to T has not been clearly identified. Nevertheless, to enable comparisons and applications to be made when small-scale yielding occurs, the results can be expressed in terms of a stress intensity-like quantity given by:

$$K = (ET*)^{1/2}$$
 (17)

where E is the elastic modulus. This can be taken as a definition of K for viscoplastic-dynamic conditions where its usual static linear elastic fracture mechanics interpretation is invalid.

A number of important points need to be considered when  $T^*$  is computed that have a significant influence on the convergence of the parameter. For small-scale yielding conditions, the stress singularity at the crack tipsee Equation (2) - results in a finite value of  $T^*$  even when the inner contour,  $\Gamma$ , is taken at the crack tip. However, because of the weaker singularity in the vicinity of the crack tip for elastic-plastic materials, the  $T^*$  integral may vanish in the limit of mesh refinement.

This can be circumvented if the appropriate definition of the elastic singularity in the region extremely close to the crack tip is achieved. Then  $T^{\ast}$  will converge to a (small) finite nonzero number. However, this procedure appears to be prohibitively expensive in the present computing environment and consequently other avenues must be pursued. Alternatively, an exclusion region can be introduced in the computation of the volume term. This is equivalent to taking the inner contour a small distance away from the crack tip. Frequently this distance is the length of the smallest element. This suggests that the  $T^{\ast}$  integral should be used in combination with some length scale such as by linking the size of the contour to some microstructural dimension of the material.

The exact form of this criterion remains to be resolved and verified; i.e., by demonstrating the transferability of the criterion from one specimen to another. Consequently, a basic issue in viscoplastic fracture mechanics is to determine a suitable parameter for the prediction of crack propagation and arrest.

# Fracture Propagation Experimentation

The experimental research is aimed at obtaining dynamic crack propagation data using two types of small scale specimens. A series of duplex A533B/4340 specimens were instrumented and tested in which crack growth was monitored on the surface of the specimen using crack gages. Crack opening displacements were measured using an eddy current transducer. Dynamic strain measurements were also obtained and used to examine the relationship between stress wave propagation and crack growth response.

An illustration of a generation mode analysis of a duplex specimen test on A533B steel at room temperature is contained in Figure 5. Figure 5(a) shows the crack length history as obtained from the crack gages. The crack length history and the load point displacement history were used as the input to a dynamic viscoplastic finite element computation. The computed  $T^*$  values, converted to K via Equation (17), are as shown in Figure 5(b).

Of most relevance in this particular application is the arrest toughness value. This was found to be 100 MPa  $\rm m^2$ . Figure 6 presents the crack arrest toughness values for A533B steel, as a function of temperature indexed to RT\_NDT, as obtained from the NBS wide plate experiments. Also shown is the curve now used in the ASME code. It can be seen that the latter is generally conservative, particularly in mandating a maximum permissible toughness of 220 MPa  $\rm m^2$ . Of most interest here, however, is the good agreement between these data and those obtained from the duplex specimen testing that can also be seen in Figure 6.

Successful testing of pressure vessel steels and other high toughness materials using small specimens is related to the ability to rapidly release a large amount of energy to the crack-tip along with loading characteristics allowing proper interpretation of the results. Conventional dynamic crack propagation and arrest toughness testing techniques using duplex specimens attempt to achieve these conditions through storage of energy in the specimen itself; e.g., through a blunted crack tip. In such approaches, the measurement capacity of the specimen is controlled by the specimen volume. Consequently, successful experiments on high toughness materials cannot even now be performed with quasi-static loading of economically sized specimens.

Progress has recently been made towards delivering large amounts of energy in a short time, as well as analyzing the specimen in the context of fracture mechanics, by considering stress wave loading through the use of Hopkinson pressure bars, Couque et al (1988). This technique, known as the coupled pressure bar (CPB) test, uses two pressure bars to store energy external to compact type specimens. The controlled fracture of an embrittled material starter specimen coupling the two pressure bars is then employed to achieve a rapid release of energy from the pressure bars to the rigidly attached specimens. The fact that two specimens can be tested simultaneously both aids in the preservation of symmetry and increases the efficiency of the experiment.

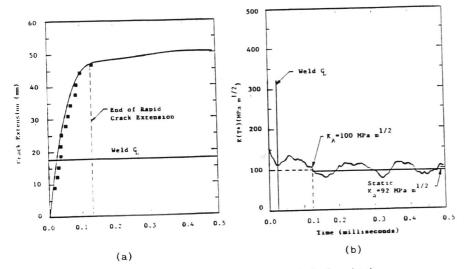


Fig. 5. Results from a 4340/A533B steel duplex test showing the  $\rm I_A$  estimation procedure a) least-squares fit to the crack extension history, b) stress-intensity factor history derived from computed values of T\*.

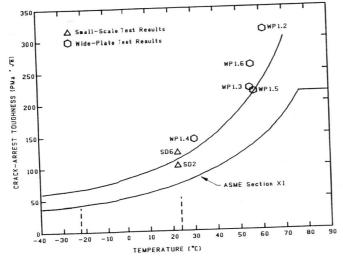


Fig. 6. Comparison of crack-arrest toughness values deduced from analyses of small-scale tests and wide-plate experiments on A533 steel.

# SUMMARY AND CONCLUSIONS

The preceding discussion has been focused on two main points. First, that a practical need exists for crack arrest fracture mechanics methodology, and, second, that fundamental dynamic fracture mechanics advances are essential to fulfilling this need. In this paper emphasis was placed upon the use of dynamic-viscoplastic treatments as a logical extension of the established elastodynamic approach. In so doing, a number of unresolved critical issues were identified as possibilities for future research. In summary, the main questions that need to be addressed are:

- 1. What is the most appropriate representation of the viscoplastic behavior of engineering materials for the ultra high strain rates that are experienced by a rapidly propagating crack?
- 2. Can a physically meaningful viscoplastic crack tip dominating parameter be identified that will provide material crack propagation/arrest properties that are independent of the computational model?
- How can the heat generated, the inelastic deformation wake, and the discrete microstructural details associated with rapid crack propagation and arrest be quantified?

As these issues surely must be addressed in the context of a balanced and well-integrated combination of careful experimentation and rigorous computational modeling, the approach outlined in this paper may serve as a model of how this can be done.

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