**AN INVESTIGATION OF THE EFFECTS
OF HISTORY DEPENDENT DAMAGE
IN TIME DEPENDENT FRACTURE
MECHANICS:
Nano-scale Studies of Damage Evolution**

To

Department of Energy
Office of Basic Energy Sciences

August, 2002

Principal Investigator: F. W. (Bud) Brust, Jr
Grant No. DE-FG02-90ER14135

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1.0 HIGH LEVEL RESEARCH PURPOSE

High temperature operation of technical engineering systems is critical for system efficiency and will be a key driver in the future US energy policy. Most systems, from new power generation schemes, innovative and/or new chemical processes, vehicle propulsion, etc., operate efficiently and reduce environmental hazards only when operated at very high temperatures. Often potential processes must be abandoned because the high temperature management costs prohibit marketplace development. Some of the newer chemical production systems, which are based on micro- or nano- tech processes, *must* operate at very high temperatures otherwise the competitive advantage compared with traditional developments cannot be realized. These new micro-tech systems are the basis for advanced fuel cells and efficient heat exchangers. President Bush's aggressive new energy policy includes an important emphasis on advanced nuclear power systems. The new generation concepts for nuclear plants rely heavily on the need for very high temperature operation – much higher than current PWR and/or BWR nuclear plants used today. Next generation aerospace vehicles will be propelled by systems that rely on very high temperature operation. Indeed, future materials for high temperature application may come from building the materials at the nanometer size scale.

Unfortunately, in this age where terrorists may strike the United States on our home soil, high temperature performance of structural systems, which experience severe damage from hostile enemies, is a new important concern. It is now known that the world trade center buildings fell after the terrorist attack when high temperature creep damage and buckling of structural members on the higher floors led to a progressive failure of the buildings rather quickly. Other vulnerable operations, such as power generation plants, chemical process plants, etc., can fail due to failures that occur at very high temperatures. Understanding the high temperature damage and failure mechanisms is critical as we develop plans and systems to thwart such attacks minimizing the damage to the systems and preventing loss of life.

Here, the focus is on understanding the high temperature deformation and damage development on the nano-scale (50 to 500 nm) level. The high temperature damage development process, especially with regard to low and high cyclic loading, which has received little attention to date, is studied. It is seen that damage development under cyclic loading develops in a fashion quite different from the constant load situation. Finally, it is noted that

failures of high temperature equipment are often catastrophic and highly publicized, and are to be avoided at all costs.

Developing an understanding of high temperature creep and creep-fatigue failure processes is a key driver for the research work described here. More importantly, the development of analytical methodologies so that high temperature management of new systems can be realized, is a key element of this work. The research efforts discussed in this report focus on both the nano- and micro- scale levels. The objectives include the development of a fundamental understanding of the deformation and failure response of structural materials that operate at high temperatures. Of particular importance is in understanding damage nucleation and growth in severe history dependent or cyclic loading at high temperature. The research in this program are providing an understanding of the high-temperature void nucleation, coalescence, crack nucleation, and crack growth process, which is a frequent dominant failure mechanism in structures that operate in severe thermal environments. A secondary objective of this work is in further understanding the effects of the welding process on failures. Indeed, most service problems and failures occur in and near welded connections for metals.

Finally, it is important to recall that high temperature life management research work was of high priority a generation ago. In the 1970's and 1980's the Department of Energy focused significant resources to develop methodologies to manage high temperature structural performance, mainly related to advanced reactor designs. Worldwide, high temperature structural research became a second order priority in the late 1980's and through the 1990's except for relatively small research programs. The exception, perhaps is Japan, which apparently continued aggressive development of high temperature creep and creep-fatigue predictive methodologies. Current methods to predict and manage life of structural components, which operate under creep-fatigue conditions, require a huge database of material tests. These tests are very expensive to perform and lead to reluctance to use new materials in high temperature designs. Continued research work in the high temperature regime is critical to the US energy policy as we move into the new millennium.

2.0 INTRODUCTION

Damage nucleation, growth, and failures of metallic structural components that operate at high temperature are considered. While metals are the main focus some of the developments are equally applicable for ceramics and even some composite systems. Damage nucleation usually begins with the development of small voids at a size level at the high end of the nanoscale (50 to 500 nm). These voids begin to grow via diffusion mechanisms along the grain boundaries along with dislocation creep within the grains. Voids eventually link-up to produce micro-cracks (size 2 to 20 μm). Micro-cracks then link-up to produce macro-cracks, which eventually leads to component failure.

From recent studies and field experience it is now known that current engineering methods to predict the life and prevent failures of components that operate in these severe environments are ineffective. Very conservative design methodologies are used in conjunction with large test databases, which are very expensive to develop, because of the lack of reliable life prediction methods. This often results in costs that preclude advanced and new designs. Moreover, the use of new structural alloys is retarded because of the perceived need to develop an exhaustive

creep-fatigue database. Hence, an understanding of the high temperature cyclic response of these components, as well as a predictive life methodology, is very important to the DOE goal of providing safe and cheap energy to the USA. On the nanoscale level, cavitation along grain boundaries leads to isolated voids, which eventually link up and lead to a macro crack. The macro crack then grows until it reaches a size where ultimate failure occurs. On the nano-, micro- and macro-mechanics levels, methods to predict the response under severe history dependent loading had received little attention prior to this program. The empirical methods used in industry .

are inaccurate and require large conservative safety factors. More importantly, the link between the nanoscale level where damage nucleates and the macro level, where engineering design predictions must be made has not been adequately established, especially under cyclic loading. This link is another program goal. Finally, the effect of residual stresses and porosity caused by welding on structures that operate at high temperature has not been well understood. Since failures frequently occur in the field in and near welds, it is important to extend the understanding and models to account for weld residual stress, strain, and damage effect. By learning how to manage the high temperature structural environment the DOE goal of providing safe, cheap, and efficient energy to the US will be improved.

2.1 High Temperature Damage Progression

Damage nucleation, growth, damage link-up, crack growth, and breakage are the typical progression of failure for components that operate at high temperature. Damage nucleation begins (see illustration below) with the nucleation of a cavity at a size scale at the higher end of the nano-scale level (~ 50 to 300 nm, depending on the material). Early in the process, such nucleation and growth phenomenon is explained by diffusion of atomic flux from the cavities to the grain boundaries, along with grain boundary sliding (to a lesser extent). As time proceeds, nonlinear viscous flow (creep) occurs, and, depending on the local stress state, eventually overrides the diffusion growth process, especially as the neighboring voids approach each other. As voids link, micro-cracks develop, link-up, and lead to a macro-crack. Depending on the operating conditions, the macro-crack can slowly grow during component operation, or fail quickly. Often

failures are catastrophic with release of large amounts of energy. In addition, as we move forward in the new millennium, higher temperature chemical processes are clearly required to increase efficiencies and reduce pollution levels.

In earlier work we focused on the understanding, control, and development of predictive methodologies to manage this type of growth under severe history dependent conditions. However, the current efforts are focused on understanding the cavitation process at the high end of the nano-scale through the grain boundary scale. Indeed, control of creep failures can only be accomplished by chemical solutions at this scale, or clever 'mechanical' solutions such as control of 'residual stresses' at this level. Since few analytical efforts have focused on cyclic time dependent cavity growth at this scale, it is the main focus of our effort. A complimentary, related effort involves the development of predictive models that can be used to control failures at the macro-scale by clever control of weld residual stresses. It is now realized that weld induced residual stresses can be a major factor in life extension.

Aging of our power generation infrastructure remains an important consideration to the US economy. Often life extension plans are developed and repairs made to existing plants to permit use long past the original design life. The weld model development portion of the present work can and has been used to model and design these repairs. This requires one to model the material removal process, model the weld repair process and post-weld heat treatment, and then the life of the repair as the equipment again operates at high temperatures. This has been done and represents a 'near term' payoff of some of this research. Of course, a new concern of our power generation infrastructure from high temperatures caused by terrorist attacks is a new area of concern where these predictive methods are necessary.

The following report is structured as follows. First, a summary of the work at the nano-scale level is overviewed. Much of the work summarized represents new developments over the last year. Prior program work can be found in earlier yearly reports. Next, high temperature response at the micro-scale level is overviewed. Section 5.0 then provides an overview of the macro-scale work including weld-modeling work. Finally, a summary and needs for future work are provided along with a list of some recent publications resulting from the work.

3.0 NANO-SCALE STUDIES OF CREEP DAMAGE DEVELOPMENT

At high temperature, cavity initiation and cavity growth are important phenomena in understanding the failure mechanism and in predicting the lifetime of various parts in service in the area of power plant and aerospace application. Such nucleation and growth phenomena are explained by diffusion of atomic flux (from cavity surface to grain boundary), creep flow, and grain boundary sliding. Cavity growth leads to cavity coalescence, and then grain boundary rupture occurs. Prediction of the cavity growth rate and final grain boundary rupture time is important in estimating rupture lifetime of high temperature service material since cavity growth examination of the structure in service is difficult.

Many researchers have proposed a cavity growth rate equation numerically and compared their results with experimental data. Because of the complexity of the physical phenomenon, in most of the numerical work, one of the two extreme cases, fast grain boundary diffusion or fast surface diffusion, with or without the consideration of grain material deformation, is assumed.

However, there has not been any unified cavity growth rate analysis where the combined effects of creep flow and surface/grain boundary diffusion mechanisms on cavity growth are considered.

In this portion of the work, the grain boundary rupture process is analyzed by both single cavity and grain level approaches. In the single cavity level approach, a 'unit cell model', which contains a single cavity on the grain boundary, is used. The goal of this single cavity level approach is to develop a unified numerical method for cavity growth where combined effect of deformation and two distinct diffusion mechanisms are considered. On the grain level model, a disk without any cavity geometry represents a cavitating grain boundary facet. The description of cavity growth is provided to the model as the boundary condition of the disk through an approximate equation where the coupled influence of grain boundary diffusion and grain material deformation is considered. By employing an experimentally verified material behavior model in the grain level approach, we are able to numerically predict the grain boundary rupture phenomena of polycrystalline metal subjected to cyclic loading. The obtained results are compared to numerical predictions based on other material behavior models, and the importance of using a realistic material behavior model is demonstrated.

Given the stress state in the neighborhood of the grain boundary, the unit cell model provides detailed microscopic analysis of single cavity growth including the change in geometry and size. The grain level analysis, on the other hand, provides information on local stress state in the neighborhood of the grain boundary so that grain boundary rupture phenomena can be predicted. The goal of this work, therefore, is to establish a physically based life prediction method for high-temperature application materials.

Currently, some significant results have been obtained both in the unit cell model and the grain level approach. This research this section of the report, therefore, is separated into two sections – Sections 3 and 4.

3.1 Introduction

Because of the complex physical phenomena, in most cases of numerical analysis for cavitation by diffusion, one of the two extreme cases, fast grain boundary diffusion or fast surface diffusion, is assumed. When grain boundary diffusivity is much faster than surface diffusivity (surface diffusion controlled process), the cavity shape will be similar to a crack because the atomic flow rate along the cavity surface is not fast enough to reduce surface curvature at the cavity tip. On the other hand, when surface diffusivity is much faster than grain boundary diffusivity (grain boundary diffusion controlled process), the cavity shape will be spherical.

The basic model for predicting a grain boundary diffusion dominant cavitation process was first proposed by Hull and Rimmer [1959] (see Fig.3.1 (a)). M. V. Speight and J. E. Harris [1967] and J. Weertman [1973] included proper boundary conditions in the Hull-Rimmer model. Their model predicts cavity growth rate in the rigid surrounding material with the assumption of a grain boundary diffusion controlled process. V. Vitek [1978] calculated cavity growth rate taking into consideration the deformation of the surrounding elastic material. R. Raj [1975] considered the events occurring during the elastic transient time. However, in the above models, plastic material deformation of the grain material is neglected, and the surface diffusivity is assumed to be much faster than the grain boundary diffusivity.

W. Beere and M. V. Speight [1978] and G. H. Edward and M. F. Ashby [1979] attempted to model the combined effect of creep flow of the surrounding grain material and the grain boundary

diffusion process on cavity growth. However, in these two models, it is assumed that elastic material surrounds the cavity. Needleman and Rice [1980] established a variational principle approach for creep flow and grain boundary diffusion coupled problems and obtained a finite element solution for the cavity growth rate. Fig. 3.1 (b) shows the effect of creep flow on the grain boundary diffusion and the updated spherical cavity profile based on the assumption of fast surface diffusion.

The assumption of grain boundary controlled cavitation may not always be satisfied, and elongated rupture cavities are sometimes observed. Thus, T-J Chuang and T. R. Rice [1973], T-J Chuang et al. [1979], and G. M. Pharr and W. D. Nix [1979] analyzed the surface diffusion controlled process numerically and verified their results against the experimental data by S. H. Goods and W. D. Nix [1978] and Raj [1978].

Since the development of the variational principle approach by Needleman and Rice [1980], further research studies have been performed to analyze the combined phenomena of grain boundary diffusion and surface diffusion (Cocks [Applied solid mechanics, vol. 3], J. Pan and A.C.F. Cocks [1993,a], A.C.F. Cocks and J. Pan [1993], J. Pan and A.C.F. Cocks [1993,b], J. Pan and A.C.F. Cocks [1995], Z. Suo and W. Wang [1994] and B. Sun, Z. Suo and A.C.f. Cocks [1996]). The main problems in coupling surface and grain boundary diffusion are to satisfy three physical boundary conditions at the cavity tip, i.e., the continuity of chemical potential, equilibrium dihedral angle, and matter conservation law. The FEM diffusion element used by Cocks can be used only for rigid material when both grain boundary and surface diffusion are considered.

Despite its apparent importance, no analysis has been done on cavity growth including grain boundary and surface diffusion mechanisms and viscoplastic deformation of the grain material which all occur simultaneously. The numerical studies of these combined effects on the cavity growth will provide basic understanding of these synergies, and they will be useful in identifying the critical conditions where the combined effects become important. In this study, the effect of the ratio of the surface and grain boundary diffusivity on the cavity growth rate is examined numerically through the development of a general model which accounts for all creep mechanisms.

3.2 Methodology

The atomic flow rates are proportional to driving forces, which are chemical potential gradients of the atom. When tensile stress is applied on the grain boundary, atoms diffuse from the cavity surface to the grain boundary due to chemical potential gradient. As atoms diffuse from the cavity wall to the grain boundary, the grain should accommodate the diffused atoms. If the grain material deforms elastically or plastically, matter accommodation occurs, mainly around the cavity tip since stress concentration occurs there.

In this work, the effects of grain boundary/surface diffusion mechanisms and viscoplastic deformation of grain material on cavity growth is examined. The chemical potential of the atom on the cavity surface μ_s , and that on the grain boundary μ_{gb} respectively, are given by

$$\mu_s = -\gamma(k_1 + k_2)\Omega \quad (3.1a)$$

$$\mu_{gb} = -\sigma_n\Omega. \quad (3.1b)$$

The atomic volume, surface energy, curvature of the cavity surface, and normal stress along the grain boundary are respectively represented by Ω , γ , κ , and σ_n . The driving force for the surface diffusion denoted by F_s and that for the grain boundary diffusion denoted by F_{gb} , respectively, are given as follows.

$$\begin{aligned} F_s &= -\frac{\partial \mu_s}{\partial S} \\ F_{gb} &= -\frac{\partial \mu_{gb}}{\partial S} \end{aligned} \quad (3.2)$$

where 'S' is the curvilinear coordinate along the cavity surface and grain boundary.

Assuming the linear kinetic law, the surface and grain boundary atomic flow rates, denoted by j_s and j_{gb} , respectively, are expressed as follows.

$$\begin{aligned} j_s &= M_s F_s \\ j_{gb} &= M_{gb} F_{gb} \end{aligned} \quad (3.3)$$

where M_s and M_{gb} are given by

$$\begin{aligned} M_s &= \frac{D_s}{kT} \\ M_{gb} &= \frac{D_{gb}}{kT} \end{aligned} \quad (3.4)$$

and D_s , D_{gb} , k , and T , respectively, are the surface diffusivity, grain boundary diffusivity, Boltzman constant, and absolute temperature.

Therefore, the rate of energy dissipation due to grain boundary and surface diffusion is:

$$\text{The rate of energy dissipation} = \int_{\Gamma_{gb}} F_{gb} j_{gb} d\Gamma + \int_{\Gamma_s} F_s j_s d\Gamma. \quad (3.5)$$

The total potential energy E of the system is:

$$E = \int_{\Gamma_{gb}} \gamma_{gb} d\Gamma + \int_{\Gamma_s} \gamma_s d\Gamma - \int_{\Gamma_F} F \cdot U d\Gamma + \int_V \sigma \cdot \epsilon dV \quad (3.6)$$

where grain boundary and cavity surface free energy, respectively, are represented by γ_{gb} , γ_{gb} , and F , Γ_{gb} , Γ_s , Γ_F , and U represent, respectively, traction, grain boundary area, cavity surface area, traction specified surface, and displacement.

Among all the virtual diffusive flux fields that satisfy the matter conservation law and the virtual velocities of the nodes in the grain material, the actual velocity and flux fields minimize the functional:

$$\bar{F} = \int_{\Gamma_{gb}} \frac{j_{gb}^2}{2M_{gb}} d\Gamma + \int_{\Gamma_s} \frac{j_s^2}{2M_s} d\Gamma + \frac{dE}{dt}. \quad (3.7)$$

In this analysis, cavity growth rate and cavity shape evolution is calculated by combining Finite Element and Finite Difference Methods for a given time step. First, the Finite Element Method by Needleman and Rice [1980] is used to calculate atomic flow rate due to grain boundary diffusion and cavity shape change due to grain material deformation and 'jacking' for given cavity geometry and cavity tip stress. Second, open ended finite difference method by G.M. Pharr and W.D. Nix [1979] was used to update cavity shape for a given atomic flow rate. After cavity shape is evolved for given step time, chemical potential of atom at cavity tip is approximately calculated from the value of principal curvatures of node next to cavity tip. At the next time step, cavity tip stress is used for FEM analysis and the same procedure is repeated until cavity coalescence occurs. A Power law type material constitutive equation is assumed. Fig. 3.2 shows the structure of numerical calculation procedure.

First, the FEM formulation by Needleman and Rice is implemented to include viscoplastic material deformation and grain boundary diffusion on cavity growth. In the Needleman and Rice approach, diffusive flux along the cavity surface was not considered and the cavity shape could not be updated. A cavity profile update procedure is explained in the next FDM analysis.

Following Needleman and Rice, the functional, $\bar{F}$, is given by,

$$\bar{F} = \int \frac{n}{v^{1+n}} \Lambda \dot{\epsilon}^{(1+n)/n} dV - \int_{\Gamma_f} \mathbf{F} \cdot \mathbf{V} d\Gamma + \int_{\Gamma_{gb}} \frac{j_{gb}^2}{2M_{gb}} d\Gamma + \int_{\Gamma} \sigma_o m_{\alpha} j_o d\Gamma \quad (3.8)$$

for all kinematically associated fields, v_i, ϵ_{ij} , and j . In the above equation, m_{α} and σ_o are the unit normal to the arc (Γ) of the intersection of the grain boundary and cavity surface and normal stress at the cavity tip, respectively, as shown in Fig. 3.3 (a). j_o is the volumetric flow rate at the cavity tip. The last term comes from the boundary condition at the cavity tip, which is given by the condition of continuity of the chemical potential. If the chemical potential of the atoms at cavity tip is not continuous, flux will be unbounded at the cavity tip. Therefore, the normal stress at the cavity tip (σ_o), also known as the sintering stress of the cavity, is a function of the specific surface energy (γ_s) and cavity principal curvatures at the cavity tip (κ_1 and κ_2) to satisfy the equation

$$\sigma_o = \gamma_s (\kappa_1 + \kappa_2) \quad (3.9)$$

Since we start the analysis for the creep flow and grain boundary diffusion problem from known primary curvatures and surface energy, the last term in the above functional can be readily solved.

A cylinder containing a cavity at the center as shown in Fig. 3.4 represents the unit cell model for FE analysis. The material is assumed to be incompressible, and this leads to the velocity boundary condition on the outer boundary of the cylinder ($r = b$). Due to the symmetric geometric condition, only one quarter of the unit cell is sufficient for the analysis. The far-field stress state is assumed to be uniaxial. The remote creep strain rate in z-direction is represented by $\dot{\epsilon}_{\infty}$, and the corresponding remote stress in z-direction is denoted by σ_{∞} .

After some numerical manipulation to relate the diffusive flux along the grain boundary to the velocity of the nodes on the grain boundary, the stiffness matrix is constructed from the functional equation. (3.8). The cavity growth rate is calculated for the given stress (σ_∞), grain boundary mobility (M_{gb}), cavity tip geometry (k_1, k_2 , see Fig. 3.3(c)), and material constitutive relation. The solution of this problem gives two results: the diffusive flux (j_o) at cavity tip and the velocity of nodes along the cavity surface.

Second, the cavity evolution due to surface diffusion is solved. As discussed earlier, Needleman and Rice assumed that a spherical cavity shape was maintained during cavity growth for grain boundary diffusion controlled problem. However, experimental results (S.H. Goods and W.D. Nix [1978] and Raj [1978]) have shown that the shape of a cavity becomes a crack rather than a sphere under the surface diffusion controlled condition. Therefore, an analysis, which includes the surface diffusion process, will produce a physically more appropriate result than the Needleman and Rice result. It is proposed that the cavity profile will be updated at each time step, satisfying boundary conditions.

Fig. 3.5 (a) shows the axisymmetric spherical-shape cavity with boundary conditions at cavity top and cavity tip. Due to symmetric condition, only one quarter of the cavity is sufficient for cavity evolution simulation. At cavity top, atomic flux, j_s , and the angle, α , are zeroes because of symmetric condition. At cavity tip, the angle, α_o , is fixed by the force equilibrium condition between grain boundary and surface tension, which is

$$\alpha_o = \cos^{-1}[\gamma_{gb} / 2\gamma_s] \quad (3.10)$$

The dihedral angle (α_o , see Fig. 3.4 (b)) between the cavity surface and grain boundary should be maintained to satisfy local force equilibrium, and this condition is given as another boundary condition. The angle between two nodes at cavity tip is maintained to satisfy this local force equilibrium. If the chemical potential is not continuous at the cavity tip, matter flow from cavity surface to grain boundary cannot occur. Therefore, Eq. (3.9) is the fourth boundary condition. The principal curvatures of the node next to cavity tip are used to calculate cavity tip stress (Eq.3.9) for FE analysis at next time step.

The four boundary conditions imposed for cavity evolution are:

$$\left. \begin{aligned} \alpha &= 0 \\ J_s &= 0 \end{aligned} \right\} \text{at the top of the cavity}$$

$$\left. \begin{aligned} \alpha &= \alpha_o = \cos^{-1} \left[\frac{\gamma_{gb}}{2\gamma_s} \right] \\ (k_1 + k_2)_{tip} &= \frac{\sigma_o}{\gamma_s} \end{aligned} \right\} \text{at the cavity tip} \quad (3.11)$$

For given step time, cavity shape is evolved satisfying matter conservation law and boundary conditions.

The current Finite Difference analysis method used here is similar to G.M. Pharr and W.D. Nix [1979] open-ended finite difference method. The atomic flow driven by chemical potential difference along cavity surface, J_s , is

$$J_s = \frac{D_s}{kT} \frac{d(k_1 + k_2)}{ds} \quad (3.12)$$

where ' D_s ' is the surface diffusivity, ' k ' is Boltzmann's constant, ' T ' is the absolute temperature, and ' ds ' is surface arc element in the direction of the flux. The diffusive flux (j_o) at the cavity tip is given from previous FE analysis.

The cavity surface velocity is determined from the atomic flux gradient, which is

$$V_n = \frac{\Omega}{r} \frac{d(J_s r)}{ds} \quad (3.13)$$

for the axisymmetric case where ' r ' is the radial coordinate. Equations (3.12) and (3.13) are kinetic equations which can describe cavity evolution.

The proposed method provides a physically based cavity growth rate that considers two important aspects of the cavity growth mechanism. First, it includes the effect of elastic/viscoplastic material deformation on single cavity growth. Second, the cavity profile is updated satisfying the physical boundary conditions, i.e., the matter conservation law, equilibrium dihedral angle, and continuous chemical potential condition.

In the next section (3.3.1 and 3.3.2), the proposed numerical method is verified for two extreme cases; grain boundary diffusion controlled cavity growth or surface diffusion controlled cavity growth. In 3.3.3 and 3.3.4, cavity evolution of the initial quasi-equilibrium cavity shape is numerically analyzed and cavity growth predictions using the new numerical method is compared with experimental results.

3.3 Results and Discussion

3.3.1 Modeling of Grain Boundary Diffusion Controlled Cavity Growth

When grain boundary diffusion controls cavity growth, it is expected that initial spherical shape cavity grows maintaining its original shape. Needleman and Rice [1980] calculated cavity growth rate and final rupture time of initial spherical-shape cavity based on rapid surface diffusion assumption and Chen and Argon [1981] proposed analytical equation, which reproduce Needleman and Rice[1980] numerical results within an error of 30%. In the following, grain boundary diffusion controlled cavity growth is calculated using current numerical method and compared with numerical result of Needleman and Rice [1980] and analytical result of Chen and Argon [1981].

Needleman and Rice [1980] numerically calculated cavity growth rates for different cavity sizes and a/L values. L is length-scale parameter. They found that creep flow accelerates cavity growth. As pointed by Needleman and Rice [1980] and several authors (Beere and Speight [1978], Edward and Ashby [1979]), creep flow of surrounding grain material shortens matter diffusion distance along grain boundary. Chen and Argon [1981] found that the cavity growth rate equation matches well with Needleman and Rice [1980] numerical result if cavity half

spacing, 'b', is replaced with length scale parameter 'L' in the cavity growth rate equation. The replacement is only valid when $a+L < b$. The equation proposed by Chen and Argon [1981] is

$$\frac{\dot{V}}{a^3 \dot{\epsilon}_\infty} = 2\pi(L/a)^3 \left[\ln\left(\frac{a+L}{a}\right) + \left(\frac{a}{a+L}\right)^2 \times \left(1 - \frac{1}{4}\left(\frac{a}{a+L}\right)^2\right) - \frac{3}{4} \right]^{-1} \quad (3.14)$$

Sham and Needleman [1983] pointed out that cavity growth rate calculated from the above equation matches with Needleman and Rice [1980] numerical result within an error of about 30 % for all values of a/L less than 10.

In this study, numerical analysis of initial spherical-shape cavity growth was carried out for $D_s/D_{gb} = 171$, $a_i/b = 0.1$ and $a_i/L = 0.316$. Equilibrium dihedral angle was chosen to be 70° and creep exponent was taken to be 4.5. Fig. 3.6 shows cavity radius increase with non-

dimensionalized time, $t\dot{\epsilon}_e^{cr}$. Cavity growth rates by Needleman and Rice [1980] are only available for $a/b = 0.1, 0.2, 0.33$, and 0.66 . Therefore, cavity growth rate between these values are obtained by the interpolation method suggested by Needleman and Rice [1980]. Although they proposed extrapolation method to calculate cavity growth rate over $a/b=0.66$, it was not applied here. From Fig. 3.6, it is clear that proposed numerical method can reproduce Needleman and Rice result exactly without the assumption of fast surface diffusivity.

When 'jacking' effect is not included, present model overestimates cavity coalescence time. Therefore, it is also clear that 'jacking' effect and creep flow of surrounding grain material can cause significant difference in calculating cavity growth rate and cavity shape evolution. When Chen and Argon [1981] proposed Eq. (3.14), they assumed that grain boundary displacement (jacking effect) due to matter flow is constant over diffusion distance 'L'. However, Needleman and Rice [1980] pointed out that material accommodation occurs mainly at cavity tip when plastic deformation occurs. Also, when diffusivity ratio is between two extreme cases, grain boundary diffusion/surface diffusion dominant, cavity shape can evolve into a more complicated one, not spherical or crack-like one, due to 'jacking effect'. This effect will be more important as a/L increases due to more severe matter accommodation at cavity tip. Analytical predictions from Eq. (3.14) are similar to the current numerical result up to $a/b=0.5$. When a/b is larger than 0.5, Chen and Argon [1981] model cannot predict Needleman and Rice [1980] cavity growth rate

results correctly. Fig. 3.7 shows non-dimensionalized cavity growth rate, $\frac{\dot{V}}{\dot{\epsilon}_e^{cr} a_i^3}$, at different a/b

values. Cavity growth rate predicted by current numerical method matches well with Needleman and Rice [1980] numerical result at $a/b = 0.1, 0.2, 0.33$, and 0.66 . Chen and Argon [1981] equation underestimates cavity growth rate when $a/b > 0.5$.

3.3.2 Modeling of Surface Diffusion Controlled Cavity Growth

When surface diffusion controls cavity growth, cavities elongate in the direction of normal to the applied stress and cavity growth kinetics change. Chuang et al. [1979] studied crack-like cavity growth by solving the Nernst-Einstein surface diffusion equation. They assumed initial

crack-like cavity shape. They obtained the steady state solution for a crack-like cavity growth. L. Martinez and W.D. Nix [1981] extended the numerical work of Pharr and Nix [1979] to study cavity evolution from initial spherical shape cavity to crack-like cavity. However, both methods did not include 'jacking' effect. Also, both methods are not applicable for the analysis of cavity growth process in which material creep flow affects grain boundary diffusion and cavity shape change. In the following, cavity coalescence time predicted by current numerical method is compared with the numerical results of L. Martinez and W.D. Nix [1981] and analytical results of T-Z Chuang et al. [1979] without considering 'jacking' effect and material creep deformation.

In presenting the result, time is expressed in units of

$$t_s = \frac{a_i^4}{D_s \gamma_s} \quad (3.15)$$

and stress is expressed in nondimensional form as

$$\Sigma = \frac{\sigma a_i}{\gamma_s} \quad (3.16)$$

The diffusivity ratio is expressed as

$$f = \frac{D_b}{D_s} \quad (3.17)$$

In Fig. 3.8, a log-log plot of the rupture time vs. applied stress is shown. For $f = 1$ and $f = 10$, current numerical results agree well with the results of L. Martinez and W.D. Nix [1981] (denoted as M & N) and T-Z Chuang et al. [1979] (denoted as C & R). L. Martinez and W.D. Nix [1981] reported stress exponents for fracture as -1.7 and -2.2 for $f = 1$ and $f = 10$, respectively. The stress exponents also match well with previously reported results. Fig. 3.9 shows stress distribution along grain boundary. Since a cavity becomes crack-like as it grows, normal stress at cavity tip for $f = 10$ becomes higher than that for $f = 1$. In Fig. 3.10, it is shown that initial spherical-shape cavity changes to crack-like shape. The nodes on cavity surface were marked along cavity surface. Initially, 15 nodes existed along cavity surface with same distance. As cavity shape becomes crack-like, more nodes exist along high curvature area. From the above two results, the current numerical model is verified against two extreme cases; grain boundary/surface diffusion controlled cavity growth cases. The new model is now is used to solve new combined surface and grain boundary diffusion problems.

3.3.3 Transition from quasi-equilibrium mode to crack-like mode

Chen and Argon [1981] calculated critical cavity size at the time of transition from quasi-equilibrium mode to a crack-like mode as a function of material properties and boundary conditions. In the following, the analytical method proposed by Chen and Argon [1981] is explained briefly followed by the comparison of numerical results produced by current method with analytical results by Chen and Argon [1981].

The following equation, Eq. (3.18), shows the relation between cavity volume growth rate and matter diffusive flux at cavity tip and major radius of cavity, 'a' which is driven from the mass conservation law.

$$\frac{dV}{dt} = 4\pi a \Omega j_{s(tip)} \quad (3.18)$$

The left-hand side of the above equation can be related with Eq. (3.14), which describes cavity volume growth rate resulting from coupled grain boundary diffusion and grain material creep flow. From Eq. (3.14) and Eq. (3.18), Chen and Argon[1981] obtained the following equation.

$$4\pi a \Omega j_{s(tip)} = \dot{\epsilon}_{\infty} a^3 \left(\frac{L}{a}\right)^3 2\pi \left[\ln\left(\frac{a+L}{a}\right) + \left(\frac{a}{a+L}\right)^2 \times \left(1 - \frac{1}{4}\left(\frac{a}{a+L}\right)^2\right) - \frac{3}{4} \right]^{-1} \quad (3.19)$$

T. Z. Chuang and J. R. Rice[1973] and T. Z. Chuang, K. I. Kagawa, and J. R. Rice[1979] showed that the surface flux is only relevant with the cavity radius, 'a', and cavity radius growth rate, 'da/dt', provided cavity geometry is given and cavity growth is at a 'quasi-steady' state. T. Z. Chuang, K. I. Kagawa, and J. R. Rice[1979] related surface flux and 'da/dt' based on the above condition for quasi-equilibrium and crack-like mode respectively. The suggested equations are:

$$j_{s(tip)} = \frac{h(\psi)}{\Omega} a \frac{da}{dt} \quad \text{for the quasi-equilibrium mode and,}$$

$$j_{s(tip)} = 2 \sin\left(\frac{\psi}{2}\right) \times \left(\frac{D_s \delta_s \gamma_s}{kT}\right) \times \left(\frac{kT(da/dt)}{D_s \delta_s \Omega \gamma_s}\right)^{2/3} \quad \text{for the crack-like mode}$$

where,

$$h(\psi) = \frac{V}{\frac{4}{3}\pi a^3} = \left[\frac{1}{(1 + \cos\psi)} - \frac{\cos\psi}{2} \right] / \sin\psi. \quad (3.20)$$

Substituting $j_{s,tip}$ from Eq. (3.20) into Eq. (3.19), the growth rate of quasi-equilibrium cavity and crack-like cavity are, respectively, obtained as follows:

$$\left(\frac{4\pi h(\psi)}{\dot{\epsilon}_{\infty} a} \frac{da}{dt} \right)_{\text{quasi-equilibrium}} = 2\pi \left(\frac{L}{a}\right)^3 \left[\ln\left(\frac{a+L}{a}\right) + \left(\frac{a}{a+L}\right)^2 \times \left(1 - \frac{1}{4}\left(\frac{a}{a+L}\right)^2\right) - \frac{3}{4} \right]^{-1}$$

and,

$$\left(\frac{4\pi h(\psi)}{\dot{\epsilon}_{\infty} a} \frac{da}{dt} \right)_{\text{crack-like}} = \alpha \left(\frac{L}{a} \right)^{\frac{5}{2}} \left[\ln \left(\frac{a+L}{a} \right) + \left(\frac{a}{a+L} \right)^2 \times \left(1 - \frac{1}{4} \left(\frac{a}{a+L} \right)^2 \right) - \frac{3}{4} \right]^{-\frac{3}{2}} \quad (3.21)$$

where

$$\alpha = \left[\frac{4\pi h(\psi)}{\left[4\sin\left(\frac{\psi}{2}\right) \right]^{\frac{3}{2}}} \right] \times \left[\left(\frac{D_b \delta_b}{D_s \delta_s} \right) \left(\frac{\sigma_{\infty} L}{\gamma_s} \right) \right]^{\frac{1}{2}}$$

From Eq. (3.21), Chen and Argon [1981] calculated cavity growth rate in transition range and critical cavity size at transition time.

Fig. 3.11 shows the normalized cavity growth rate vs. normalized cavity radius. (a_i/L) and α are chosen to compare current result with analytical prediction by Chen and Argon [1981]. When $(a_i/L) = 0.1$ and $\alpha = 10$, Fig. 3.11 (a), cavity shape changes from spherical-shape to cavity-like shape with similar cavity growth rate predicted by Chen and Argon [1981]. Current numerical analysis predicts slightly faster cavity growth rate when transition occurs. Chen and Argon [1981] compared cavity growth rate equations of two extreme cases to get cavity growth rate in transition region. In reality, it is expected that cavities evolve from spherical-shape to crack-like shape gradually. Therefore it is reasonable that faster cavity growth rate is predicted during transition. When creep flow effect on cavity growth increases, such as $(a_i/L) = 0.316$ and $\alpha = 5.82$, Fig. 3.11 (b), and $(a_i/L) = 1.0$ and $\alpha = 1.0$, Fig. 3.11 (c), cavity growth rate predicted by current numerical analysis is slower than the prediction by Chen and Argon [1981]. It is explained as follows. Since 'jacking' effect and cavity shape change due to creep flow are expected to become more severe as (a_i/L) increases, cavity growth rate is decreased and cavity shape transition does not even occur in Fig. 3.11 (c). Fig. 3.12 and Fig. 3.13 shows cavity aspect ratio variation and cavity shape evolution in case of Fig. 3.11 (c). Cavity aspect ratio increases and cavity shape becomes V-shaped. Arai, M. et al. [1996] reported cavity shape evolution from quasi-equilibrium shape to V-shape under load controlled cyclic test. They argued that sharp creep strain rate increase upon stress reversal or accumulated plastic strain can be a possible reason. Under load controlled cyclic condition, grain material experiences sharp creep strain rate increase, which increases creep flow effect on cavity growth. Numerical analysis under cyclic loading conditions has not been done here but is planned. However, current numerical result shows that initial spherical cavity can evolve to V-shape depending on diffusivity ratio and a/L even when dominant cavity growth mechanism is creep flow assisted atomic diffusion.

3.3.4 Comparison of numerical prediction of diffusional growth of cavities with experiments

Goods and Nix [1978] studied cavity growth of silver with prior implanted water bubbles. They recorded fracture time t_f and fracture strain ϵ_f for each test at several temperatures between 200°C and 550°C. They also reported a correlation, $t_f \sim \sigma^{-3.7} \exp(Q/RT)$. Goods and

Nix [1978] interpreted their results based on the Chuang and Rice [1973] surface diffusion controlled cavity growth model.

However, as pointed by Chen and Argon [1981], surface diffusion controlled cavity growth condition is not satisfied in all experimental conditions. Chen and Argon [1981] compared their analytical results with Goods and Nix [1978] experimental results. They argued that, since testing time in Goods and Nix [1978] experiment was too short, it is appropriate to express cavity growth rate $\frac{4\pi\gamma h}{\epsilon a} \frac{da}{dt}$ in terms of fracture strain. They also used initial conditions of

$a_f = \frac{b_o}{4} = 1.1\mu\text{m}$, and $a_i = 0.785\mu\text{m}$. Goods and Nix [1978] first reported these quantities and

Pharr and Nix [1979] corrected to these values later. For creep strain rate, $\dot{\epsilon}$, Chen and Argon [1981] used $\frac{\epsilon_f}{t_f}$, because steady state creep rate was not reached in Goods and Nix [1978] experiments. They reported that creep strain rate from these assumptions are several orders of magnitude higher than the steady state creep rate.

Several authors reported physical constants for silver, and Table 1 shows those constants. For surface diffusion constants, its values are uncertain. In this study, Goods and Nix's [1978] physical constants were used to calculate α and a_i/L values. The corresponding values for numerical calculation were shown in Table 2.

Since $\frac{4\pi\gamma h}{\epsilon a} \frac{da}{dt} = \frac{4\pi\gamma h}{\epsilon_f} \ln \frac{a_f}{a_i}$, Chen and Argon [1981] could plot $\frac{4\pi\gamma h}{\epsilon a} \frac{da}{dt}$ vs. $\frac{a_i}{L}$.

However, Chen and Argon [1981] ignored capillarity stress, which is 0~0.4 values in this experimental condition. In this study, cavity growth rate was obtained assuming $a_i/L = 0.1$, $\alpha = 16\sim 24$, and $\sigma_o = 0 \sim 0.8$. The two branches for chosen α and σ_o values bracket experimental results well in Fig. 3.14 showing the validity of the present new model.

3.4 Conclusions

In this study, a combined numerical method, which combines Finite Element Analysis and Finite Difference analysis, was proposed. It was verified against two extreme cases; grain boundary diffusion controlled cavity growth and surface diffusion controlled cavity growth. When extremely fast surface diffusivity is given, current numerical method predicts that the cavity maintains initial spherical cavity shape, which was assumed by Needleman and Rice [1980] numerical method. In the opposite condition, that is surface diffusion controlled cavity growth, the current method successfully describes cavity shape changes from initial spherical shape to crack like shape. Although, in this method, the node next to cavity tip was used to calculate cavity tip normal stress, it was good approximation under physically reasonable diffusivity ratio. Also, it has been shown that cavity shape change is a complicated function of material diffusivity ratio, a/L , and cavity tip geometry. When creep flow effects on cavity growth is important, 'jacking' at cavity tip can affect overall cavity shape and final rupture time. Under those circumstances, the proposed numerical method can be powerful tool to predict cavity shape changes and final rupture times in the regime of creep flow assisted diffusion cavity growth.

Table 1

γ_s	ψ	T_m	Ω	D_{bo}	Q_b	Temp.	δ_b	D_{so}	Q_s	Temp.	δ_s
J/m ²	De g.	K	m ³	m ² /sec	J/mole	K	m	m ² /sec	J/mole	K	m
1.14 *	70*	1234*	1.71E- 29*	1.2E- 5*	90016.2 *	623- 753*	5E- 10*	2.5E-06 ¹ 4.5E-06 ² 1.4E-06 ³	84500 ¹ 49100 ² 67400 ³	470- 770*	2.57E- 10*

- * S.H.GOODS & W.D.NIX, Acta metall, 26, 739, 1978,
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2 T.Z.CHUANG et.al. Acta metall, 27, 265, 1979
3 N.A.Gjostein, Diffusion Seminar, ASM, Cleveland 1974

Table 2

Tem p	D_s/D_{gb}	stress	t_f	ϵ_f	$\dot{\epsilon}$	L	α	a/L	$\sigma_o\sigma_\infty$
K		Pa	Hr.			m			N/m ²
823	2.40E- 01	1.38E+ 06	3.07E+ 05	0.006	1.95E- 08	1.07E- 05	1.62E+ 01	0.073	1.98E+0 0
823	2.40E- 01	1.38E+ 07	1.35E+ 02	0.019 4	1.44E- 04	1.19E- 06	1.71E+ 01	0.660	1.98E-01
673	2.35E- 01	6.89E+ 06	7.70E+ 04	0.006 3	8.18E- 08	4.58E- 06	2.39E+ 01	0.172	3.96E-01
673	2.35E- 01	4.48E+ 07	5.62E+ 01	0.027 1	4.82E- 04	4.73E- 07	1.96E+ 01	1.660	0.61E-01
573	2.38E- 01	1.09E+ 07	3.42E+ 05	0.011 5	3.36E- 08	2.97E- 06	2.41E+ 01	0.264	0.25E-01
573	2.38E- 01	8.68E+ 07	1.85E+ 01	0.007 2	3.89E- 04	2.62E- 07	2.02E+ 01	2.995	3.15E-02
473	2.51E- 01	2.17E+ 07	3.96E+ 05	0.012 6	3.18E- 08	1.07E- 06	1.99E+ 01	0.733	1.26E-01
473	2.51E- 01	6.89E+ 07	3.31E+ 03	0.014	4.23E- 06	3.08E- 07	19.0228 8	2.545	0.04

Fig. 3.1 (a) Hull-Rimmer type diffusion flow along cavity surface and grain boundary. The grain boundary separates as rigid bodies, and (b) The effect of creep flow on grain boundary diffusion. The deformation of grain material cause local accommodation at the cavity tip.

Fig. 3.2 Illustration of numerical calculation structure with Finite Element method and Finite Difference Method.

(a)

(b)

(c)

Fig. 3.3 (a) sintering stress and unit normal vector at cavity tip (b) equilibrium dihedral angle definition (c) principal curvature at cavity tip.

$$\text{On } z = h: T_z = \sigma_{zz\infty}, T_r = 0$$

$$\text{On } r = b: T_z = 0, v_r = -\frac{1}{2} \dot{\epsilon}_{\infty} b$$

$$\text{On } r = 0: u_r = 0.$$

Fig. 3.4 Unit cell model with spherical cavity with radius 'a' and outer grain boundary radius 'b'.

Fig. 3.5 (a) Boundary condition of finite difference method (b) Schematic representation of the discretized cavity surface used in the finite difference method (c) Definition of the surface normal at the node on cavity free surface (d) Finite difference numerical scheme showing how points on cavity surface.

Fig 3.6. cavity growth vs. time, $a/L=0.316$, $a_i/b=0.1$.

Fig 3.7. Comparison of cavity growth rate prediction.

Rupture time(in units of t_s) $t_s = \frac{a_i^4}{D_s \gamma_s}$

Applied stress(in units of γ_s/a_i) $\Sigma = \frac{\sigma a_i}{\gamma_s}$

Fig. 3.8 Grain boundary rupture time vs. applied stress, $a_i/b=0.1$, cavity tip angle= 70° .

Normalized stress

Fig. 3.9 Normal stress variation during cavity growth.

(a)

Fig. 3.10 Evolution in the cavity shape, (a) $f=1$, (b) $f=10$

(b)

Fig. 3.10 Evolution in the cavity shape, (a) $f = 1$, (b) $f = 10$.

Normalized growth rate

$$4\pi h(\psi) \frac{da}{dt} / \epsilon_{\infty} a$$

(a)

$$\alpha = 10$$

$$\left(\frac{a}{L}\right)_{\text{initial}} = 0.1$$

$$\sigma_0 = 0$$

Normalized growth rate

$$4\pi h(\psi) \frac{da}{dt} / \epsilon_{\infty} a$$

(b)

$$\alpha = 5.82$$

$$\left(\frac{a}{L}\right)_{\text{initial}} = 0.316$$

$$\sigma_0 = 0$$

Fig. 3.11 Growth rate of initial spherical-cap shape cavity.

$$\alpha = 1.0$$

$$\left(\frac{a}{L}\right)_{\text{initial}} = 1.0$$

$$\sigma_o = 0$$

(c)

Fig. 3.11 Growth rate of initial spherical-cap shape cavity.

Fig. 3.12 Cavity aspect ratio variation during transition from quasi-equilibrium shape to crack-like shape.

Fig. 3.13 Cavity shape evolution from quasi-equilibrium shape to diamond shape, $a/L=1$, $\alpha=1$.

Fig. 3.14 Comparison of numerical prediction of diffusional growth of cavities with experiments (S.H.GOODS & W.D.NIX, Acta metall, 26, 739, 1978).

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4. THE EFFECT OF CYCLIC LOADING ON GRAIN BOUNDARY RUPTURE TIME: MICRO-MECHANICS MODEL

4.1 Section Overview

This section studies intergranular creep failure of high temperature service material under a stress-controlled unbalanced cyclic loading condition. The grain boundary rupture process was numerically analyzed using Tvergaard's axisymmetric model. The present numerical model incorporated the experimentally verified Murakami-Ohno cyclic strain hardening creep law and Norton's creep law. The numerical results show that cavity growth accelerates under cyclic loading condition. Also, analysis shows that a steady state creep law is not sufficient to analyze damage evolution under cyclic loading conditions.

4.2 Introduction

At high temperature, cavity initiation and cavity growth are important phenomena in understanding the failure mechanism and in predicting the lifetime of various parts in service for power plant and aerospace applications. Such nucleation and growth phenomena are explained by atomic diffusion, creep flow of surrounding material, and grain boundary sliding. Cavity growth leads to cavity coalescence, and then grain boundary rupture occurs. Prediction of the cavity growth rate and final grain boundary rupture time is important in estimating rupture lifetime of high temperature service material since cavity growth examination of the structure in service is difficult.

The axial stress applied at single cavity growth models is assumed to be same as the remotely applied stress. However, Dyson [2] pointed out that when cavitation occurs at an isolated grain boundary, as shown in Fig. 4.1 (a), the cavity growth is constrained by the creep strain rate of the surrounding material. This implies that the stress around the grain boundary can be different from the remotely applied stress due to the grain material creep flow behavior. Rice [3] successfully illustrated the constrained cavity growth phenomena and Riedel [4] and Tvergaard [1] extended Rice's work. A recent study by M. Arai et al. [5] has shown that the grain boundary rupture time can be better predicted by the constrained cavity growth rate equation than by that the Hull-Rimmer model. This constrained rate equation is a modified Hull-Rimmer equation based on Dyson's [2] concept. M. Arai et al. [5] also verified that cavity growth rate predictions based on the Hull-Rimmer model were faster than the experimental results.

In this work, the effect of cyclic loading on grain boundary rupture process is numerically analyzed using grain boundary rupture model first proposed by Tvergaard [1]. Tvergaard [1] proposed the grain size level model shown in Fig. 4.1 to simulate the constrained cavitation process at the isolated grain boundary. A disk without any void geometry represents a cavitating grain boundary facet. The description of cavity growth is provided to the model as the boundary condition of the disk through an approximate equation where the coupled influence of grain boundary diffusion and grain material deformation is considered. Tvergaard [1] used Norton's power law equation as a material constitutive equation. However, cavities can grow in the primary creep region, and cavities may already exist before the polycrystalline metal is placed in service. In addition, a significant creep strain rate can be introduced around the crack tip or

cavity upon reversing the stress state (F.W. Brust [6]). Therefore, under cyclic loading condition, constitutive equations, which describe the primary creep region, should be used to examine the cavity growth behavior properly.

Murakami-Ohno [7] proposed a continuum mechanics-based constitutive law to describe the primary creep region (see Appendix A). The notion of a creep-hardening surface is used to model a sharp creep strain rate upon stress reversal resulting from the remobilization of immobilized dislocations.

Motivated by this phenomenon, the effect of physically-based constitutive model and that of the cyclic loading history on the cavity growth was numerically simulated based on a grain size level FEM model (Tvergaard [1] model).

The results obtained will be compared to numerical predictions based on other material behavior model, and the importance of using a realistic material behavior model will be demonstrated.

4.3 Methodology

In Fig. 4.1 (a), a polycrystalline material with isolated cavitating grain boundary is shown. In Fig. 4.1 (b), periodically arrayed cavities on the grain boundary are shown. The cavity growth rate ($\dot{V}$) of each cavity is related to the straight grain boundary displacement rate ($\dot{\delta}$). In Fig. 4.1 (c), the grain size FEM model is shown. The actual cavities on the grain boundary are not modeled in this model. The initial radius of the cavitated grain boundary is denoted by d_i , and the initial height and width of the axisymmetric model are denoted by H_i and W_i , respectively, where W_i represents half of the length between two adjacent cavitated facets. The cavities on the grain boundary are assumed to maintain quasi-equilibrium spherical-cap cavity shape. The cavity growth rate can be calculated by an analytical equation as follows.

$$\dot{V} = 4\pi D_{gb} \frac{\sigma_n - (1-f)\sigma_o}{\ln(1/f) - (3-f)(1-f)/2} \quad (4.1)$$

where

$$f = \max \left(\left(\frac{a}{b} \right)^2, \left(\frac{a}{a + 1.5L_{gb}} \right)^2 \right)$$

$$L_{gb} = \left(\frac{D_{gb}\sigma_n}{\dot{\epsilon}_{cr}} \right), L_{\infty} = \left(\frac{D_{gb}\sigma_n^{\infty}}{\dot{\epsilon}_{cr}} \right)$$

where D_{gb} is the grain boundary diffusion parameter, σ_n is the normal stress, σ_o is the sintering stress, $\dot{\epsilon}_{cr}$ is the creep strain rate, 'a' is the cavity radius, 'b' is cavity half spacing, and L_{gb}, L_{∞} are diffusive length calculated above grain boundary and at the remote, respectively. The approximate cavity growth rate equation $\dot{V}$ is based on the work of Rice [3], Sham and Needleman [8], and Needleman and Rice [9]. Budiansky, Hutchinson, and Slutsky [10],

Needleman [8], and Needleman and Rice [9]. Budiansky, Hutchinson, and Slutsky [10], Tvergaard [1] proposed cavity growth rate equation due to creep flow. In this work, the cavity growth rate equation due to creep flow is ignored since it does not play a significant role in the total cavity growth rate in the constrained diffusive cavity growth range.

At each time step, the cavity growth rate (equation (4.1)) is calculated using the normal stress and the creep strain rate value of the elements at each 'cavity' location along the grain boundary. This cavity growth rate is related to the grain boundary displacement rate by the mass conservation law, as suggested by Rice [3]:

$$\dot{\delta} = \frac{\dot{V}}{\pi b^2} - \frac{2V}{\pi b^3} \dot{b} \quad (4.2)$$

This grain boundary displacement is a boundary condition of the next time step. The ABAQUS [11] commercial package is used, and the nonlinear geometric effect is considered. The Murakami-Ohno constitutive equations are implemented through the UMAT subroutine in ABAQUS. In this analysis, two types of material creep flow rules are applied and results for each case are compared. First, Murakami-Ohno strain hardening creep flow law and Norton's steady state creep flow rule are simply added to calculate total creep strain rate (denoted as 'MO + N' case). Second, Norton's steady state creep flow rule is used to calculate total creep strain rate (denoted as 'N' case).

4.4 Results and Discussion

The material properties of the 1.25Cr-0.5Mo steel at 538°C employed in this work are summarized in Table 1. Fig. 4.2 compares the creep strain predictions by the present numerical analysis with experimental data. As shown in Fig. 4.2, the Murakami-Ohno constitutive law can predict the experimentally obtained sharp creep strain rate upon stress reversal.

The present numerical analysis assumed that cavities are initially present along grain boundary. Initial cavities are assumed to be distributed along the grain boundary with the initial conditions (a_i/b_i) = 0.1 and b_i/d_i = 0.1. Remote normal stress applied is specified by $\sigma_\infty/E \approx 1 \sim 4E-4$ depending on a_i/L_∞ values and $a_i/L_\infty = 0.01, 0.015, 0.03$ and 0.05 . In this a_i/L_∞ range, dominant cavity growth mechanism is atomic diffusion assisted by material creep flow. However, when a_i/L_∞ is less than 0.05, normal stress is constrained due to slow grain material deformation. Therefore, a_i/L_{gb} , which is used to calculate cavity growth rate, is much less than a_i/L_∞ and dominant cavity growth mechanism is grain boundary diffusion. The reference time used here is defined as

$$t_r = \frac{\sigma_\infty}{E \dot{\epsilon}_{cr}} \quad (4.3)$$

It is assumed that grain boundary rupture is attained when a/b value reaches 0.65. The initial cavity tip angle is assumed to be 70° and sintering stress is taken to be zero. Fig. 4.3 shows the stress controlled loading condition applied for this analysis. The compressive loading time (t_c) is about $0.001t_f$ and t_f/t_c is 10, 50, and 100, respectively. Fig. 4.4 ~ 4.6 show normalized cavity radius increase with time for $a_f/L_\infty = 0.01, 0.015, \text{ and } 0.03$, respectively. Grain boundary displacement caused by cavity growth is not constrained when a_f/L_∞ value exceeds 0.06. Grain material starts to constrain cavity growth immediately after external loading is applied for every case. Since grain material deforms initially according to fast Murakami-Ohno creep flow law for 'MO+N' case, constraint process progresses more slowly for 'MO+N' case than 'N' case. As shown in Fig. 4.4 ~ 4.6, the effect of cyclic loading history on grain boundary rupture time is not significant for 'N' case. However, it is clear that cyclic loading condition accelerates grain boundary rupture for 'MO+N' case. Fig. 4.7 shows the stress development around the cavity located at the grain boundary center ($x_1/d=0$) for $a_f/L_\infty = 0.01$. The important aspect in this figure is the normal stress decrease due to grain material constraint. Initial grain material deformation rate difference causes normal stress difference. After transition time, normal stress saturates at the same stress value for two cases. The transition time is approximately $0.5t_f$, which is same as the transition time from primary creep region to secondary creep region for this case. Fig. 4.8 shows normal stress variation after loading transition from compression to tension at $t/t_f \cong 0.1, 1.6$ for $a_f/L_\infty = 0.01$. After stress transition, initial high normal stress around cavity decrease to normal stress under constant loading condition for both cases. The initial tensile stress value after stress transition is larger for 'MO+N' case than 'N' case under cyclic loading condition. Sharp creep strain rate increase after load reverse, as shown in Fig. 4.2, alleviates material constraint.

Fig. 4.9 shows the relation between the number of cycles and cavity coalescence time. Time to cavity coalescence for each cyclic loading case is normalized against cavity coalescence time under constant loading case. The number of cycles is obtained as follows

$$\text{Number of cycles} = t_f (\text{constant loading}) / (t_f + t_c) \quad (4.4)$$

where t_f is the cavity coalescence time under constant loading condition and t_f and t_c are tensile and compressive loading time, respectively.

Cavity shrinkage during compressive loading time is assumed to be small because of small time interval. Total cavity coalescence time decrease up to 15% under cyclic loading condition. This analysis did not include fatigue effect, grain boundary sliding, cavity growth due to creep flow, and surface diffusion. Tvergaard [12] showed cavity at grain boundary edge could grows faster than cavity at grain boundary center when free grain boundary sliding is included in the model. Including grain boundary sliding into this model is remained as future work. Also, instead of using an analytical equation for the cavity growth rate such as Eq. (4.1), more realistic cavity growth model can be included to account the effect of grain boundary/cavity surface diffusion and elastic viscoplastic material behavior on the grain boundary rupture time.

Under cyclic loading condition, the total life of the structure in service can be shorter than predicted by any of the existing life prediction models. Since most structures in service are

subjected to cyclic loading, the obtained results are significant. Additional results and more model details can be found in last years report and some of the references listed in Section 7.

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Norton's constants		Murakami-Ohno's constants			Young's modulus	Yield stress
A (MPa ⁻ⁿ hr ⁻¹)	n	A	M	N	E (Mpa)	σ_y (Mpa)
4.49E-20	8.0	7.9E-15	0.55	5.66	140.6E+03	131.0

Table 4.1 The material property of 1.25Cr-0.25Mo steel at 538°C.

Fig. 4.1 (a) Isolated cavitated grain boundary in the polycrystal (b) cavities on the grain boundary (c) Axisymmetric FEM model and boundary condition.

Fig. 4.2 Verification of ABAQUS UMAT code based on Murakami-Ohno constitutive equation with the experimental result.

$$t_r (\text{reference time}) = \frac{\sigma_e}{E \dot{\epsilon}_e}$$

t_t : loading time

t_c : unloading time ($t_c < 0.01 t_r$,
to see the effect of the cyclic loading)

t_m : transition time ($t_m \approx 0$)

Fig. 4.3 Stress-controlled remote loading condition.

(a)

(b)

Fig. 4.4 Damage evolution during unbalanced cyclic loading, $a/L=0.01$, (a) cavity at grain boundary center, (b) cavity at mid-point between grain boundary center and edge.

(a)

(b)

Fig. 4.5 Damage evolution during unbalanced cyclic loading, $a/L=0.015$, (a) cavity at grain boundary center, (b) cavity at mid-point between grain boundary center and edge.

(a)

(b)

Fig. 4.6 Damage evolution during unbalanced cyclic loading, $a/L=0.03$, (a) cavity at grain boundary center, (b) cavity at mid-point between grain boundary center and edge.

Normalized σ_e, σ_n

Fig. 4.7 Development of the stress state around the cavity at grain boundary center with the initial $a/L=0.01$ for constant loading condition.

Fig. 4.8 Normal stress variation after stress transition from compression to tension.

(a)

(b)

Fig. 4.9 Effect of number of cycles on intergranular failure time, (a) cavity at grain boundary center, (b) cavity at mid-point between grain boundary center and edge.

5.0 MACRO-SCALE STUDIES OF CREEP DAMAGE DEVELOPMENT

Welds and Residual Stress Effects. A new constitutive law that is appropriate for weld modeling has been developed. This new law accounts for weld and base metal melting, softening, and history annihilation, among many other effects that are critical for proper weld modeling. The constitutive law makes weld analyses very rapid, and this basic methodology has been transferred to industry in the form of practical and accurate weld analyses to control distortions and residual stresses. This model is being used to investigate creep life extension procedures for aging power plants by using hot compression. Similar ideas will be studied in relation to nanoscale void growth reduction. A key issue addressed here is the effect of history dependent loading on welded joints.

Details of this work are presented as part of a recent paper that is included as Appendix B. This details history dependent failure analysis work and provides references that further describe the macro-scale studies that are part of this program.

6.0 DISCUSSION AND CONCLUSIONS

Polycrystalline materials exposed to high temperature creep conditions develop voids along the grain boundary. The rate of growth of these voids depends on the nucleation mechanisms, on the initial void shape and size, the applied stress state and material behavior. Ultimate failure of the damaged material is caused by the coalescence of these voids. Studies on void growth are critical in developing appropriate life-prediction methodologies for materials exposed to high temperature creep conditions. In most metals, in addition to contribution to void growth due to creep deformation, contributions to void growth also come from grain boundary diffusion and surface diffusion. We have performed studies at the nano- and micro- scales to investigate these phenomena. This section discusses conclusions related to the nano- and micro-mechanics studies of creep and cyclic creep damage development that we have performed over the last several years of this program. This summary also discusses some of the work completed last year and correlates the results with new results of this year.

For void growth that occurs predominantly *due to creep*, it was shown in our recent work [11-16] (see Section 7 references) that void shape changes that occur during growth have a pronounced influence on the growth rates. Thus, to capture correct trends of void growth finite geometry changes need to be accounted for. In most of the studies on void growth material elasticity is considered to be insignificant and thus ignored. However we have found that elasticity effects may be an important consideration during void growth in materials experiencing cyclic creep conditions. In addition material elasticity plays a dominant role in the interaction of voids in elastic-plastic materials. The results on void growth rates and void shape changes when elasticity is ignored confirm the conclusions arrived by Needleman *et al*. The present work has also shown that except for large initial volume fractions in a creeping solid, exposed to very high triaxialities, the effect of material elasticity on the evolution of void shape and growth is very minimal. Though the void growth rates are somewhat higher for the large initial void volume fraction in a creeping solid exposed to very high triaxialities when elasticity is included, it is

unlikely to impact the total time to failure because the growth rates are very high. Additionally, the elastic transient time during void growth is found to be quite negligible for all the cases considered.

Of particular interest is the fact that certain metals experience intergranular cavitation under balanced cyclic loading conditions. Several attempts have been made to explain the phenomenon of intergranular void growth under balanced cyclic loading. A good discussion on these various attempts can be found in Reidel's book. The present results unequivocally demonstrate that material elasticity does not play any significant role in void growth under balanced cyclic loading. Rather nonlinear shape changes that occur during the balanced cycling process are an important consideration in explaining this phenomenon. This is not surprising since nonlinear shape changes significantly affect the void growth and interaction even under constant stress conditions. The calculations reveal that the cavity growth rate under balanced cycle loading is constant over the number of cycles performed. Interestingly, this observation is consistent with the experimental findings of Baker and Weertman, who show that cavity growth rate is constant in copper experiencing balanced cyclic loading at 678 K. The effect of including a correct constitutive law, such as Murakami-Ohno, will further affect this conclusion as seen in Section 4 here.

For diffusion-dominated processes, our results have predicted faster cavity coalescence than the existing models. Under cyclic loading conditions, void growth rates accelerate since the polycrystalline grains accommodate diffused material much faster than under constant loading condition. The total life of the structure in service therefore can be shorter than predicted by any of the existing life prediction models. Since most structures in service are subjected to cyclic loading, the obtained preliminary results are significant.

This prior work was extended over the last year to investigate all aspects of diffusion growth with the development of a general model. A combined numerical method, which combines Finite Element Analysis and Finite Difference analysis, was proposed. It was verified against two extreme cases; grain boundary diffusion controlled cavity growth and surface diffusion controlled cavity growth. When extremely fast surface diffusivity is given, current numerical method predicts that the cavity maintains initial spherical cavity shape, which was assumed by Needleman and Rice numerical method. In the opposite condition, that is surface diffusion controlled cavity growth, the current method successfully describes cavity shape changes from initial spherical shape to crack like shape. Although, in this method, the node next to cavity tip was used to calculate cavity tip normal stress, it was good approximation under physically reasonable diffusivity ratio. Also, it has been shown that cavity shape change is a complicated function of material diffusivity ratio, a/L , and cavity tip geometry. When creep flow effects on cavity growth is important, 'jacking' at cavity tip can affect overall cavity shape and final rupture time. Under those circumstances, the proposed numerical method can be powerful tool to predict cavity shape changes and final rupture times in the regime of creep flow assisted diffusion cavity growth. It remains to investigate cyclic load effects on diffusion creep damage development. In particular, for surface controlled diffusion where the voids flatten out, cyclic creep loading is expected to severely accelerate void growth rates. The key point is that the model, because of its generality, can be used to investigate creep damage development on the nano-scale level so as to aid in high temperature life design and analysis of high temperature structures. Finally, we would like to add the final piece to the model, which is grain boundary sliding to the model.

7.0 PUBLICATIONS RELATED TO THIS WORK

In excess of fifty five publications consisting of Journal publications, rigorously reviewed Conference publications, Symposia proceedings, and oral presentations have been made resulting fully or partially from this work over the years. Rather than list all of them here, the reader is referred to the References listed in this section and the many references cited therein. In addition, there are two papers nearly complete to be sent to journals before the end of December 2002, dealing with the nano model discussed here. Finally, there will be at least one paper submitted dealing with the micro model. The developments of the weld models continue to be used to solve engineering problems and results papers continue to be written regarding this work.

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9.0 FUTURE WORK NEEDS

Additional work will focus on the numerical study of high-temperature creep damage evolution, especially on single cavity growth and grain boundary rupture. The main objective of this additional effort is to deal with detailed numerical studies to understand stage 2 damage processes. In addition, creep flow driven cavity growth mechanism with consideration of matter diffusion and will further study grain boundary rupture phenomena by paying particular attention to the cavity shape evolution.

9.1 The effect of diffusion and creep flow on grain boundary cavitation

In the last year's work, detailed numerical study on the effect of grain boundary/surface diffusivity ratio and material creep flow on single cavity growth mechanism produced interesting results. The numerical method proposed last year could handle creep flow assisted diffusive cavity growth in which a/L are less than 10.0.

When material creep flow dominates cavity growth, $a/L > 10.0$, it was usually assumed that surface diffusion is fast enough to maintain spherical cavity shape. However, last year's result shows that cavity evolution and cavity growth rate are totally different with the previously published analytical result depending on diffusivity ratio even when a/L is less than 10.0.

We plan to investigate the cavity evolution and cavity growth rate when cavity growth is mainly driven by creep flow of surrounding material with consideration of diffusivity ratio. Based on the last year's numerical method, a more robust numerical module will be developed. From this study, it is expected that we can obtain physically more realistic cavity growth result when creep flow dominates cavity growth.

9.2 The effect of diffusivity ratio and cyclic loading on grain boundary rupture

As shown in the last year's result presented here, grain boundary rupture is a complicated phenomenon. Grain boundary/surface diffusivity, material creep flow, normal stress along grain boundary, and grain boundary sliding are key factors that decide grain boundary rupture time. There have been several numerical methods proposed to simulate grain boundary rupture phenomena. In this proposed effort, new grain boundary rupture model will be developed, which will include the effect of diffusivity ratio on diffusion/creep flow controlled cavity growth, based on Tvergaard's grain boundary rupture model.

In Tvergaard's model, two analytical cavity growth rate equations are used to calculate cavity growth; diffusion dominant growth and creep flow dominate growth. Both analytical equations were obtained with the assumption of fast surface diffusion. However, as discussed in the last year's result on single cavity growth, cavity shape can evolve to crack-like or V-shaped depending on grain boundary/surface diffusivity ratio. Also, when service material is under cyclic loading condition, creep flow around cavity has sharp increase upon stress reversal.

It is expected that new grain boundary rupture model will be developed in which grain boundary/surface diffusion, creep flow of surrounding material, and grain boundary sliding effect on cavity growth are included.

9.3 Nano-Studies of diffusion under cyclic loading

It remains to investigate cyclic load effects on diffusion creep damage development. In particular, for surface controlled diffusion where the voids flatten out, cyclic creep loading is expected to severely accelerate void growth rates. The key point is that the model, because of its generality, can be used to investigate creep damage development on the nano-scale level so as to aid in high temperature life design and analysis of high temperature structures. Finally, we would like to add the final piece to the model, which is grain boundary sliding to the model.

Appendix A

Murakami-Ohno law

Appendix A: Murakami-Ohno law

The creep strain rate by Murakami-Ohno is given by:

$$\begin{aligned}\dot{\varepsilon}_{ij} &= \frac{3}{2} m A^{\frac{1}{m}} q^{\frac{m-1}{m}} \sigma_e^{\frac{n-m}{m}} S_{ij} \\ q &= \rho + \left[\frac{(\varepsilon_{ij}^c - \alpha_{ij})}{\sigma_e} \right] S_{ij}\end{aligned}\quad (A.1)$$

where

σ_e : effective stress

S_{ij} : deviatoric stress

A, m, n : material constants

The evolution equation for the center of the yield surface α_{ij} and radius ρ are given by:

$$\begin{aligned}\dot{\alpha}_{ij} &= \frac{1}{2} (\dot{\varepsilon}_{ij} \eta_{kl}) \eta_{kl} ; \quad \dot{\rho} = \frac{1}{\sqrt{6}} \dot{\varepsilon}_{ij} \eta_{ij} \quad \text{if } g = 0 \quad \text{and} \quad \frac{\partial g}{\partial \varepsilon} \dot{\varepsilon}_{ij} > 0 \\ \dot{\alpha}_{ij} &= \dot{\rho} = 0 \quad \text{if } g < 0 \quad \text{or} \quad \frac{\partial g}{\partial \varepsilon_{ij}^c} \dot{\varepsilon}_{ij} \leq 0\end{aligned}\quad (A.2)$$

Where η_{ij} is the outward normal vector to CHS (Creep Hardening Surface) defined as

$$\eta_{ij} = \frac{\varepsilon_{ij}^c - \alpha_{ij}}{\left\{ (\varepsilon_{kl}^c - \alpha_{kl}) - (\varepsilon_{kl}^c - \alpha_{kl}) \right\}^{1/2}} \quad (A.3)$$

The CHS is given as

$$g = \frac{2}{3} (\varepsilon_{ij}^c - \alpha_{ij}) (\varepsilon_{ij}^c - \alpha_{ij}) - \rho^2 = 0 \quad \text{on CHS and } < 0 \quad \text{inside.} \quad (A.4)$$

Therefore, the radius and center of the CHS change only when the creep strain state is on the CHS and remain the same when the state of creep strain is inside the CHS. This constitutive equation can express the rapid creep strain rate increase upon stress reversal. The advantage of this theory is the fact that material constants for classical strain hardening constitutive theory can be used. Reference 7 describes more details of the model and the numerical implementation.

Appendix B

The Importance of Material Fabrication History on Weld Durability and Fracture

Frederick W. Brust¹

The Importance of Material Fabrication History on Weld Durability and Fracture

Reference: Brust, F. W., "The Importance of Material Fabrication History on Weld Durability and Fracture", *Fracture, ASTM STP 1644*, W. G. Reuter and R. S. Piascik, Eds., American Society for Testing and Materials, West Conshohocken, PA, 2001.

Abstract: Fabricated metallic structures originate as plate stock at the material manufacturer. The residual stresses in the plate stock depend on the steel manufacturing process and the heat treatment and cooling methods applied. The residual history is then carried through and is altered by the cutting, bending, welding, etc. required for the fabrication. This process can create additional residual stresses and/or will alter the residual stress or distortion throughout the parts and components. As will be seen, by the time the material from the steel plant makes its way into the service structure, each component has already seen a history of stresses, nonlinear strains, and corresponding displacements. This history can have an important effect on the service life of the structure. Fatigue, corrosion cracking, fracture, etc. can all be affected by prior history. However, in most cases this prior history is neglected in design or when making a damage assessment of the structure. *Fatigue and fracture assessments are often made by pretending that the service material is pristine, free of prior fabrication history effects.* The fatigue life, corrosion response, and final fracture behavior predicted assuming a pristine structure can be different from that which would be predicted by including prior history.

This paper illustrates the effect of prior history on weld-fabricated structures through the use of several examples. The fatigue behavior, the corrosion response, and the final fracture behavior for several cases where history effects are included are compared to predictions where these effects are neglected. Guidelines for determining when prior fabrication effects must be included in the design and life management process are provided. Finally, simple methods for accounting for these in the design and life management cycle are overviewed.

Keywords: residual stresses, welds, weld fabrication, fracture, weld modeling.

Critical components of fabricated structures that are operated in critical applications are often stress relieved before service life begins in an effort to eliminate prior history effects. However, the costs associated with stress relief are often not justifiable for many applications. However, in some instances, neglecting the effects of the fabrication history can reduce the accuracy of the life prediction. Such fabrication residual stresses can have an important effect on corrosion life, fatigue life, fracture resistance, creep damage, and local constraint.

This paper attempts to investigate the effects of fabrication history on failures. The paper first illustrates how fabrication residual stresses can be introduced into a structure. Next, a new

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computational weld model is overviewed. This weld model is used in some examples that are provided later in the text. Next we provide several case studies which illustrate fabrication effects life.

Material History Dependence

Structures continually degrade during the service performance years. Initial fabrication flaws (especially for welded fabrication) may be present, fatigue and corrosion cracks may initiate and grow, etc. Assuring that these defects do not lead to service failures is an important goal for the product manufacturer and the structural fabricator. Structural integrity can be ensured by assuming the presence of flaws at highly stressed regions of the structure and performing fatigue, corrosion, and fracture analyses of the structure under service conditions. In addition, when flaws are found in service, the repair schedule (timing, type of repair, etc.) can be determined by performing such a fracture assessment.

Usually damage assessments are made by neglecting prior history in the components that make up fabricated structures. Consider the cycle represented by Figure 1 for a fabricated steel structure. Start from the upper left and move clockwise. The different components may be cast, rolled, forged, etc. from the material supplier, and often combinations are used in the service structure. An initial residual stress and distortion pattern develops depending on which process is used. For instance, in rolled plate, tensile stresses usually develop near the plate edges and compressive stresses develop in the interior.

The rough material stock is then transported from the steel mill to the fabrication shop. The transportation, handling, and storage may alter the original stress and deformation history inherent in the rough stock. The material may then be surface treated, depending on the application, further altering the original history in the rough stock. The material is then cut into the desired shape required for the fabrication (for instance, consider a truck frame consisting of a number of components (forged, cast, rolled) and welded together). This cutting process alters the original residual stress history (and thus distortion history). Moreover, the cutting process may induce additional residual stresses near the cut edge (particularly for thermal cutting since the thermo-mechanical flame cutting process induces nonlinear strains near the cut edges).

The component might then be bent and formed into the required shape for the fabrication. Forming again alters the original history, and can add additional significant stresses and strains in the bent regions of the component. Connecting the parts with welds, bolts, adhesives, etc. assembles the different components into the desired structure. The connection process further alters the residual history in the component parts.

Figure 1 - Operations History Leading to Structural Fabrication.

In particular, the welding process induces significant residual stresses and distortions into the assembled structure. Finally, the assembled component or structure might then be straightened to achieve certain desired tolerance requirements. This process further alters the history in the structure.

As seen, by the time the material from the steel plant makes its way into the service structure, each component has already seen a history of stresses, nonlinear strains, and corresponding displacements. As an example, consider Figure 2. This is an example of the effect that bend forming and welding on the service residual stress state for a mild steel. As illustrated on the left of Figure 2, a two-dimensional nonlinear finite element analysis was performed of a plate being bent in a die. Next, a weld bead was deposited on the exterior of the bend curvature. Both the bending and welding processes were modeled via the finite element method (the weld models used are described next). The right side shows black and white contour plots of the 'X' component of stress (this component will likely lead to crack growth at the weld toe). The material was a standard structural steel. The stress magnitudes vary between + and - 300 Mpa (the magnitudes are not important for our purposes). It is clearly seen that stresses at the weld toe are markedly different between the two cases.

This history can have an important effect on the service life of the structure. Fatigue, corrosion cracking, fracture, etc. can all be affected by prior history. However, in most cases this prior history is neglected in making a damage assessment of the structure. *Fatigue and fracture assessments are often made by pretending that the service material is pristine, free of history.* The fatigue life predicted assuming a pristine structure is different from that which would be predicted by including the prior history (welding alone (Figure 2 (a) or bending and welding 2(b)). References [1-5] further illustrate this point and a examples will be shown later that clearly illustrate this effect.

Of course, for some critical structures, stress relief of many of the components is performed before the structure goes into service. However, the costs associated with stress relief are not practical for the vast majority of fabricated structures. In addition, 'stress relief', annealing, and other processes do not eliminate all residual stresses and strains leading to a pristine structural component.

Because residual stresses caused by the welding process are often dominant compared with other fabrication induced stresses, and because many service failures occur at welds, we spend some time discussing the state-of-the-art of weld process models before providing examples.

Figure 2 – Bending and welding effects on residual stress development.

Computational Weld Model

Background - Perhaps the first attempt to predict the residual stresses induced by the welding process was carried out by Rodgers and Fletcher [6] in 1938 using an analytical approach. A number of other analytical approaches were developed from this time through the early 1970's to predict distortions and residual stresses (see for instance the survey paper by Masubuchi [7]). These approaches were quite novel and often provided reasonable predictions when compared with experimental measurements, but were often limited to single pass welds.

Such analytical approaches were replaced by numerical approaches in the early 1970's as the power of the finite element method was realized. The earliest published finite element models developed for predicting the residual stresses induced by the weld process were probably developed independently by Kamichika et al in Japan [8] and Friedman [9] in the USA. Battelle researchers (References [10-14]) extended these models in the late 1970's and early 1980's to account for (among other features) multiple pass welds, material re-melting and annealing, phase changes and heat sinks. The Battelle work was also perhaps the first to use closed form analytical solutions to develop accurate high speed weld thermal analysis procedures for finite thickness (including thin) plates. These models were used extensively in studies for the nuclear power industry to develop weld procedures to mitigate inter-granular stress corrosion cracking in piping systems. Methods such as Heat Sink Welding (HSW - Reference [13]), Induction Heating for Stress Improvement (IHSI - Reference [14]), and Backlay Welding (BW - Reference [10]) were developed and optimized using these models and these methods are still used in the nuclear industry. As such, this work probably represented the first industrial application of a weld process model to solve a manufacturing problem.

Since 1990 weld process models have been developed and are being used by several different organizations. References [15, 16, 17, and 18] summarize methods used by organizations in Germany, Canada, USA (Edison Welding Institute), and Austria, respectively, to model weld induced residual stresses and distortions. No attempt to summarize the methods used by these and other organizations is attempted here; rather the interested reader can consult these references and references cited therein and below for details.

In the early to mid 1990's the present authors in conjunction with Caterpillar, Inc., began to greatly improve all of these weld analysis tools. In particular, the high-speed thermal solution procedures and the structural procedures such as local annealing, melt element detection, etc., (References [6-10]) were extensively updated and improved for the nuclear industry, the aerospace industry, the Department of Energy, the automotive industry, among others. References [19, 20] describe these developments for thick plate nuclear applications, Reference [21] describes this work for thin plate aerospace applications using advanced metals, Reference [22] describes some of the theoretical developments of the model improvements in recent years (developed with by DOE funding), and Reference [23] describes automotive applications.

The Weld Process Model

Model Overview - Since this early work, a number of researchers have developed weld

process models or used commercial finite element codes to perform weld analyses. Most commercial codes were not specifically developed to properly account for the many unique features of the welding process. Some of these unique features which must be accounted for include: proper thermal heat flux input, melting/re-melting effects, history annihilation as temperatures are between the phase change temperature and melting, and slow solution speed. The model used here overcomes these deficiencies.

Figure 3 - *Weld Process Model Illustration.*

The model components are illustrated in Figure 3. As seen, there are two parts to the model.

Thermal Model - Analytically based methods and numerical (finite element or finite difference) methods are used to predict the temperature versus time histories in the weld piece. Numerical solutions based on the finite element method, the finite difference methods, control volume techniques, etc., can always be used to obtain the temperature versus time profiles throughout the history of the structure being welded. However, numerical solutions often require extensive manpower and computer resources to analyze complex structures. Analytically based solutions have been developed which are extensions of the 'Rosenthal type' [24] methods discussed in references [10-14]. The recently developed advanced versions of analytical solutions can account for radiation and convection losses, weld torch start/stop effects, complex weld geometry's, transient effects, among others. *These are very high-speed solutions, which permit analyses of huge structures to be performed rapidly and quite accurate for many applications.* References [25-28] and references sited therein provide some details of these new solutions.

Thermal Model Verification - The analytically based thermal analysis procedures have been verified through a number of comparisons with numerical solutions and with experimental measurements. A large library of verification solutions on component geometry's such as lap and Tee-fillet joints and on full-scale large structures has been compiled. Here we provide an example validation for a T-fillet weld as seen in Figure 4. Figure 4 shows a T-fillet weld in 12 mm thick plate. The comparisons between thermocouple measurements (designated 'Exp') and analysis (designated 'Cal') are shown in these figures. In addition, the ABAQUS thermal solution procedure, in conjunction with a USER DFLUX routine is used where very accurate local temperatures are required. This procedure permits the weld heat input to the piece to be accounted for via a 'modified Goldak' double ellipsoidal approach [16, 28].

Figure 4 - Analytical Thermal Model Prediction Compared With Experiment. The weld direction is shown and TC-1 is 0.5 mm and TC-2 is 4.5 mm From the Weld Toe. TC-2 represents a location near the stop point of the weld. This illustrates that the complicated 'start/stop' procedures are working well. TC-1 is a location very close to the weld toe.

Structural Model - Unfortunately, there are many unique features associated with the welding process that cannot be correctly nor efficiently modeled using ABAQUS (or other general purpose finite element packages) unless a number of user written features and utilities are added to the weld analysis procedure. In particular, the library of material models (or constitutive laws) available in ABAQUS cannot account for some of the unique features

associated with the welding process (Figure 5). This includes history annihilation* caused by melting/re-melting as different weld passes are deposited, material phase changes, and thermal cycling, among others. Moreover, the procedures required to model the weld process using ABAQUS are quite awkward. For instance, when modeling the weld process using the finite element method, the weld metal ahead of the current arc position has not been deposited as yet. To correctly account for this effect using ABAQUS one must use a tedious element birth option. This procedure is tedious in terms of manpower requirements and is computer intensive.

To overcome these problems, user interface constitutive subroutines have been written. These interface with ABAQUS to account for the unique features associated in a physically meaningful way. In addition, some the procedural difficulties discussed above as well as solution speed are overcome by using these constitutive routines. Reference [22] provides details of the constitutive law used for weld modeling.

Stress Validation - Figure 6 illustrates an example of the accuracy expected with the weld process model. This shows an example of a lap fillet welded circular plate welded to a larger plate. The residual stresses were measured using X-ray diffraction along the radial line plot illustrated in the Figure 6 inset. This represents a location 180 degrees from the weld torch start/stop position. The range of experimental data for the radial stress plot represents two separate measurements. It is seen that very good predictions

Figure 5. *Mathematical structure of a weld material routine*

* By "history annihilation" here we refer to the loss of deformation history (such as plastic strains and stresses) that occur when material is heated to temperatures greater than about 70 percent of melting (or near the phase change temperature). One may think of this definition as a sort of 'local' stress relief.

Figure 6 – One example of weld model validation for stresses.

are made. Observe from Figure 6 that tensile radial and hoop residual stresses develop from the welding process in the region adjacent to the weld toe. It is these stresses that can be reduced or made negative that can greatly increase the fatigue life of a structure. The stress predictive capability of the model has likewise been extensively verified for many different weld geometry's, including complex cases as well. As with temperatures, an extensive library of weld model validation examples exists. In addition, extensive library's of distortion prediction validation cases exists.

The weld model has been incorporated into a software package called VFT[®] (Reference [29]). This code has been used extensively over the past several years to develop weld strategies to eliminate distortions and control residual stresses for a variety of large-scale structures. Some examples are provided in References [30-33]. As with stresses, control of distortions can have an important effect on reducing fabrication costs. This weld process model is an important tool used in achieving these objectives.

Examples

Fracture of Welded Beams

Following the 1994 Northridge earthquake, wide spread damage was discovered in the pre-qualified welded steel moment frames. Detailed inspections indicated that most of the structural damage occurred at the weld connections between the beam and column flanges. In particular, the weld joints between the bottom beam flange and the column face suffered the most severe damage. Cracks mostly initiated at the weld root and propagated with very little indication of plastic deformation. The desired plastic hinges assumed in the structural building codes 'plastic design' were not formed in the weaker beam away from the weld joint. Instead, brittle weld fracture was identified as the dominant failure mechanism.

Welding-induced residual stresses are believed to be one of the factors contributing to the brittle fracture. Indeed, there exist ample evidence that residual stresses can play dominant role in the fracture process of highly restrained welded joints (References [34,35]). The design of welded moment resistant frame connections presents perhaps the most severe mechanical restraint conditions both during welding and in service. Consequently, the presence of high weld residual stress is expected. In addition, the triaxiality of the residual stress state in these joints can be significant. As such, the anticipated plastic deformation cannot develop before the fracture driving force reaches its critical value, resulting in brittle fracture.

Figure 7 illustrates an analysis of a typical beam-column connection (A36 beam, A572 Gr. 50 column, and E70T-4 weld material). The inserts illustrates the three dimensional cross section of the finite element mesh that was used to model the welds in the beam-column. In addition, a two dimensional model was used as well. The residual stresses (not shown here – see Reference [36]) showed a very high degree of triaxiality and were directly caused by constraints induced by the welding process and the geometry. The two-dimensional mesh illustrated below the beam column (Figure 7) was used to study the fracture response of a typical lower flange in a beam column connection. Nine passes were deposited (see inset mesh of Figure 7). The stress intensity factor is plotted as a function of the ratio of applied tensile stress to weld yield stress in the right of Figure 7. It is seen that including the history of residual stresses in the analysis procedure has a marked effect on the stress intensity factor. Indeed, for fracture in the brittle or transition regime, including prior history in the analysis is critical to obtain correct results.

Car Body Frame

The example illustrated above in the beam-column connection weld joint illustrated that weld induced residual stresses not only increase the stress intensity factor but can also increase the constraint. This can result in lower failure loads than those predicted without including residual stress effects. However, there was no attempt in the above case to develop weld procedures to eliminate or minimize these the deleterious effects caused by the welding itself.

There are a number of ways to modify the welding process to either control distortions or to manage residual stresses. These include weld sequence definition, pre-

Figure 7 – Residual stress effects on fracture for a beam-column connection.

cambering, pre-bending, heat sink welding, thermal stretch welding, heat input control, weld torch travel speed, among many others. The present example illustrates how a service-cracking problem was eliminated by a simple weld sequence change that was determined via VFT analyses.

Consider a 'swivel frame' in a large off road mining vehicle as in Figure 8. The finite element mesh to the left represents an axisymmetric model of a cylinder welded to a base plate via a Tee-fillet weld. Field cracking was observed in the vehicle, and it sometimes occurred immediately after the weld. The cylinder is quite large with a diameter of 3.5 meters and a thickness of 33 mm while the base plate has a thickness of 100 mm. The original weld sequence is illustrated in the top of Figure 8 and labeled 'sequential'. This led to the type of cracking illustrated in the inset, where the cracks initiated in the cylinder at the inner diameter, near the toe of the weld, through the cylinder.

Since the thickness of the welded parts is large, it was postulated that constraint was a possible cause of the cracking. As such, the VFT code was exercised in an attempt to develop a weld sequence that might eliminate the problem. After several iterations, the sequence illustrated in the bottom portion of Figure 8, labeled 'alternating' was determined to minimize both the constraint and the weld residual stress state. This

Figure 8 – Carbody weld sequence example.

sequence consists of welding at the inside diameter first, followed by the outer diameter, then inner diameter, outer diameter, etc., until the weld is complete. The residual stress state that develops from the two sequences is illustrated in Figure 9. Here it is seen that the stresses near the toe of the weld are markedly higher with the original sequence compared with the sequential sequence. In addition, though not shown here, the constraint for the alternating weld was also significantly lower than the sequential weld. This new sequence was implemented into the shop floor of the manufacturer and not one failure has been observed since. This is an example that illustrates how clever design and control of fabrication induced residual stresses can eliminate field failures.

Figure 9 – Residual stresses from sequential and alternating welding.

Storage Tank Welds

Welded steel storage tanks are used in many industries. The weld sequences of these tanks can have an important effect on how cracks initiate and grow. Consider

Figure 10 – Typical Weld sequence for large storage tank and analysis mesh.

Figure 10. Large storage tanks are typically fabricated by vertically and horizontally welding sections of curved plate. Here the effect of the weld intersection on subsequent corrosion driven crack growth is considered. The tank was considered to have a large radius to thickness ratio so that the finite element model, illustrated in the right half of Figure 10, was made flat. For this example, the horizontal weld (labeled 'H' in Figure 10) was laid first, followed by the vertical weld (labeled 'V' in Figure 10). Both welds were double-V groove welds with 6 passes

modeled per weld and the plate thickness was 12.7 mm. VFT was used to predict the initial residual stress state in the tank. A symmetry plane was assumed along the vertical weld line and the dimensions and boundary conditions chosen so as to eliminate 'edge' effects.

Within and near the weld intersection area, the residual stress distributions are rather complex due to the interactions of the two welds. The high longitudinal residual stress of the horizontal weld (in the direction of weld 'H') is significantly reduced at the weld intersection due to the subsequent introduction of the vertical weld. The heating and cooling process induced by the deposition of the vertical weld passes relieves the longitudinal stresses of the horizontal weld in intersection area. After completion of the vertical weld, the residual stress (in the direction of weld 'H') distribution at the intersection is dominated by the transverse residual stress component of the vertical weld. The same observation can be made for the distribution of the stress in the vertical weld direction (in the direction of the 'V' weld), where the longitudinal residual stress of the vertical weld dominates the vertical residual stress distribution at the intersection region. In effect, the last weld dominates the residual stress characteristics at the intersection area.

One important consequence of the interaction effects between the horizontal and vertical welds is that the resulting tensile horizontal residual stresses (in the 'H' direction) are increased in both magnitude and area at the intersection region along the side of the vertical weld. (Note that if the weld sequence is reversed, a large tensile vertical residual stress region will occur at the intersection region along the horizontal weld.) The presence of such a tensile residual stress region will certainly impact the stress intensity factor solutions if the horizontal residual stresses become operative for a crack situated along the vertical weld in this region. Such effects on stress intensity factor solutions are discussed next.

Cracks are introduced into the residual stress regions near the intersection of the welds as illustrated in Figure 11. The finite element alternating method (FEAM) (see for Figure 11 –

Crack Locations for stress intensity factor calculations.

instance Reference [37]) was used to calculate the stress intensity factors for the different crack sizes considered. FEAM is quite convenient for this application since stress intensity factors are readily evaluated using the mesh of Figure 10 directly, i.e. no special crack specific finite element mesh is required. Figure 12 shows the stress intensity factors as a function of crack size for cracks located along both the vertical and horizontal

Figure 12 – Stress intensity factors for vessel intersection welds.

welds. For the vertical cracks it is seen that the weld residual stresses in the 'H' direction are the major contributor. K increases as the crack size increases up until about a crack size of about 2.5 inches after which it continually decreases as the crack increases in size. Moreover, the cracks are expected to grow more at both the inner and outer vessel surfaces compared with the mid surface (here we are concerned with 'K' driven stress corrosion crack growth).

For the horizontal cracks, K decreases from an initially large value for small cracks until it appears to reach a steady state value, independent of crack size. The crack at the inner and outer surfaces are expected to grow more so than at the mid plane. These results suggest that the

cracks, if driven mainly via the residual stress field, may grow to a rather large size at the inner or outer surface of the vessel before breaking through the vessel wall. It also suggests that the horizontal cracks may grow without bound if the steady state K-value is higher than the threshold for SCC growth.

Leak-Before-Break Issues In Piping Systems

An important consideration in leak-before-break (LBB) analysis for nuclear piping system is an accurate prediction of crack-opening area (COA). A comprehensive discussion on this subject can be found in Rahman et al [38]. Among some of the important issues, effects of weld residual stresses on crack-opening behavior are not well understood. A comparative study using the special shell element discussed earlier and an elastic superposition method was reported Reference [38], where it was demonstrated that a full-field residual stress field can introduce more significant crack closure than predicted using the elastic super-position method.

As the through-wall crack becomes longer, present LBB procedures Reference [38] assumes the crack opening area becomes proportionally larger, according to linear elastic analysis results. Consider a 406 mm diameter welded pipe with an R/t ratio of 10 and $t = 16$ mm (typical of nuclear piping). As shown in Figure 13, the actual circumferential crack opening behavior becomes rather complicated once the full field weld residual stresses are considered. As the crack length increases from $2c = 150$ mm to 300mm and 500mm, the crack opening profile starts to deviate from the typical elliptical shape, particularly at ID and crack closure effects become more significant. Such non-elliptical opening behavior can be attributed to the increasing effects of the hoop residual stresses along the crack face as the crack increases in length. Accordingly, crack opening area calculations must take such effects into account for LBB assessment.

More importantly, it is seen that the crack opening profiles are negative at the outer diameter (OD) and mid surface (MS). The through wall axial weld residual stress distribution for this pipe (and typically for this thickness pipe) is tension at the ID and compression at the OD. Of course, this is physically impossible, but it clearly suggests that crack closure (or pinching) of the crack may occur restricting leak flow rates. As such, leak rate detection equipment may not detect leaks as designed for. Since these calculations did not include service loads (only weld induced residual stresses are considered), the cracks in service are expected to be open. For thinner wall pipe, the effect of residual stresses on crack leak rates can be important. This is the subject of an ongoing effort to develop correction factors to account for weld induced crack closure for LBB considerations.

Distance from Crack Front (mm)

Distance from Crack Front (mm)

Distance from Crack Front (mm)

Figure 13 – Crack opening displacements in pipe with different crack sizes.

Discussion

This paper provided an overview of some of the issues of concern regarding material fabrication histories. It is now clear that solution to service failures (distortion, corrosion, fatigue, creep, etc.) can be made earlier in the fabrication chain. For instance, if the plate stock material is provided with known (and consistent) residual stress and distortion states, distortion correction issues that may be required at the final stage of fabrication can be eliminated. The use of computational models to address each step of the fabrication process is critical.

Four examples were provided in this paper that illustrates some of the important features associated fabrication and residual stresses. Constraint and residual stresses caused by welding can lead to reduced service lives and unexpected failure modes. A number of additional examples can be cited. For instance, creep damage control of weld repairs can be designed via computational models (Reference [39]) and post weld heat treatments. Repair of damaged pipes can be designed using computational models (Reference [40]). Numerous other examples are cited in the reference list as well.

In our view, the question of fabrication history dependent fracture, including weld fracture where residual stresses and strains are important, is very much open. New fracture parameters that perform and are verified in this regime are needed.

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