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MASTER

MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS

by

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SUMMARY

The work performed during the past fiscal year included in the materials area:

1. The development of microstructural basis for a second generation state variable deformation model.
2. The continuation of the work on a unified model for grain boundary anelasticity and grain boundary sliding.
3. The continued investigation of the grain boundary cavitation process in the Zircalloys.
4. The application of a state variable approach in materials characterization.

in the mechanics area:

1. A finite element analysis of thermal stress transients in structures.
2. The application of the boundary element method to plate bending and fracture.

INTRODUCTION

The work performed during the past year is a part of the continued effort at Cornell University to establish a state variable description of non-elastic deformation and related phenomena in crystalline solids and to develop applications to mechanical design.

For completeness this report contains also the work in the mechanics area performed during the period September 1, 1979-August 30, 1980 under Contract No. DE-AS02-76ER02733. Since September 1, 1980 the above contract was combined with the present contract.

An important development of the past year has been in the area of establishing the microstructural basis of the grain matrix processes for our state variable deformation models. Progress in this area was enhanced by our work on the second generation deformation model (1). The second generation model assumes the existence of barriers to dislocation motion with varied strength instead of barriers with uniform strength assumed by the original model proposed by Hart (2). This new assumption is physically more realistic and allows direct correlation between the materials parameter of the model and the dislocation microstructure observed by electron microscopy. We are encouraged by our progress. It appears that we shall be able to develop, based on the observed correlations, microstructure based theories to support our phenomenological models.

Our work in this general area has been motivated in part by our concern that there are many seemingly unrelated theories and correlations for non-elastic deformation. Many of these theories and correlations were justified based on rather limited experimental data. In order to remedy this situation, we believe that an important first step should be to broaden the experimental data base from which we can identify the common and systematic behavior exhibited by different materials. The expanded data base should provide us with an opportunity to construct phenomenological models which will describe a wide variety of deformation phenomena in a unified manner. We also believe that once the phenomenology of deformation processes is well defined, we shall be in a better position to correlate deformation properties with microstructural observations and to develop physically based theories.

We have not taken the approach preferred by some of the investigators in this field, that is to propose a dislocation based theory or model first and then perform experimental work to verify the theoretical predictions. We feel that non-elastic deformation involves complex processes such that a mainly theoretically based approach may not be completely satisfactory. Fortunately during the past ten years we have been supported and have developed efficient mechanical testing methods which enabled us to accumulate the required data base. Based on our experimental data we have been able to construct state variable phenomenological models of general applicability. The correlation established during the past year between the materials parameter of the model and dislocation structure represents the first step in a new direction

for our research. We plan to pursue actively the development of microstructure based theories for our model and to account for the effects of thermal-mechanical history. Work in this new direction will be an important part of our effort. We shall, of course, continue to emphasize in our research the application of our state variable approach in materials characterization and in mechanical design.

Grain boundary anelasticity and grain boundary sliding is another area of materials work where significant progress was made. In the previous progress report (3) we described our attempt to develop a unified description of these two phenomena. Grain boundary anelasticity in our work is considered to result from grain boundary sliding accommodated by elastic and anelastic deformation of the grain matrix at grain boundary corners, steps and at second phase particles in the grain boundary. Grain boundary sliding as a plastic deformation process will involve accommodation by grain matrix plastic deformation at the same sites. We have proposed three models of increasing complexity to describe both phenomena. During the past year we have been able to develop computer simulation programs based on these models and have applied them successfully. Experimentally we have performed load relaxation tests on polycrystalline nickel specimens and obtained experimental data which reflect the contribution of grain boundary sliding. We are presently using nickel data, both the load relaxation data and the closed stress-strain loops, obtained under conditions where grain boundary effects are important to determine

the level of complexity required in model development.

In the work on the grain boundary cavitation during creep in the Zircalloys, we are continuing our effort to collect cavity nucleation data as a function of temperature, applied stress and creep strain. This is a laborious task but a necessary one.

The rate of creep cavity nucleation is expected to depend on the magnitude of stress concentration at grain boundary corners, steps and at second phase particles in the grain boundary as a result of deformation incompatibility produced by grain boundary sliding. The temperature dependence of the extent of grain boundary sliding in plastic deformation is not a simple monotonic function. We do not expect therefore that the temperature dependence of creep cavity nucleation will be a simple one. A large test matrix covering a wide range of important variables will be necessary in order to allow us to assess the complete picture of creep cavity nucleation.

In other areas of materials work we have used our state variable approach for materials characterization to obtain information of engineering interest. We have used the load relaxation test to investigate the effects of texture on the flow properties of the Zircalloys for the purpose of optimizing the cladding properties of LWR fuel pins. This research was a joint project with EPRI. We have also worked with Hanford Engineering and Development Laboratory to use state variable constitutive equations to simulate the deformation behavior of cold worked Type 316 stainless steel thin walled tubes under a variety of loading conditions. As

a part of the latter work. We have developed constitutive equations which can be used to describe deformation properties during recrystallization. We have been able to use the same set of constitutive equations to simulate tube creep data which involved long testing times as well as temperature transient data which involved short testing times and rapid rate of temperature change at temperatures where recrystallization occurred.

In the mechanics area in addition to continuing our effort to improve the efficiency of our computational capabilities for mechanical design, we began to investigate also problems which will have more direct metallurgical interests.

There are a variety of phenomena in materials science and in metallurgy where time dependent mechanical effects are present. Because of the complexity in geometry, in materials property and in experimental condition involved in these problems, simplified assumptions are often made in their analysis. For example, the rate effect is usually not considered in calculating the plastic zone size at a crack tip. With the computational capabilities and the constitutive equations developed in our research program, we should be in a good position to take a further look at some of these problems.

During the past year, we have analyzed the problem of cavity growth at elevated temperatures by creep under an internal pressure. In our calculation we have accounted for realistically the effects of stress redistribution and work hardening. Our results showed a significantly different time dependence of cavity

growth rate compared to that obtained based on steady state creep (4). The latter type of analysis has been made recently by several investigators. This difference will necessitate a change in the interpretation of the kinetics data of hydrogen attack in carbon steels (5).

We have analyzed also the fracture problem and developed the computational capabilities for plastic deformation at the crack tip. We are able to calculate the evolution of plastic zone at the crack tip as a function of loading rate. We should be in an excellent position to incorporate current fracture theories in our analysis and to examine the significance of their predictions.

In the following we shall report the progress made in various areas during the past year in separate sections. The reports written during the same period are listed below.

1. R. L. Keusseyan and Che-Yu Li, "Precision Strain Measurement at Elevated Temperatures Using a Capacitance Probe," accepted for publication in ASTM Journal of Testing and Evaluation.
2. R. L. Keusseyan, J. Wanagel, H. Ocken, J.T.A. Roberts and Che-Yu Li, "The Effect of Fabrication Variables on the Load Relaxation Behavior of Unirradiated Zircaloy Sheet," submitted to the Journal of Nuclear Materials.
3. C. W. Cho, P. Alexopoulos, M. S. Jackson and Che-Yu Li, "A Phenomenological Model for Transient Deformation Based on State Variables II: Experimental Verification," submitted for publication in the Journal of Engineering Materials and Technology.
4. P. S. Alexopoulos, G. L. Wire, H. Yamada and S. Mukherjee, "A State Variable Analysis of Inelastic Deformation of Thin Walled Tubes: I Modelling," submitted for publication to the Journal of Engineering Materials and Technology.

5. G. L. Wire, D. R. Duncan, N. S. Cannon, G. D. Johnson, P. S. Alexopoulos and Che-Yu Li, "A State Variable Analysis of Inelastic Deformation of Thin Walled Tubes: II Data Analysis and Simulations," submitted for publication in the Journal of Engineering Materials and Technology.
6. M. Morjaria and S. Mukherjee, "Finite Element Analysis of Time-Dependent Inelastic Deformation in the Presence of Transient Thermal Stresses," accepted for publication in the International Journal for Numerical Methods in Engineering.
7. M. Morjaria and S. Mukherjee, "Inelastic Analysis of Transverse Deflection of Plates by the Boundary Element Method, ASME Journal of Applied Mechanics, Vol. 47, p. 291 (1980).
8. S. Mukherjee and M. Morjaria, "A Boundary Element Formulation for Planar Time-Dependent Inelastic Deformation of Plates with Cutouts," International Journal of Solids and Structures (in press).
9. M. Morjaria and S. Mukherjee, "Numerical Analysis of Planar, Time-Dependent Inelastic Deformation of Plates with Cracks by the Boundary Element Method," International Journal of Solids and Structures (in press).
10. S. Mukherjee and M. Morjaria, "Boundary Element Analysis of Time-Dependent Inelastic Deformation of Cracked Plates Loaded in Anti-Plane Shear." Submitted for publication in the International Journal of Solids and Structures.

STRUCTURE-PROPERTY RELATIONS

In this section we shall report the effort made in the characterization of the dislocation structure in Type 316 stainless steel and in establishing the relation between microstructure and the materials parameter of our phenomenological model. The parameters examined included the hardness parameters and microplastic and anelastic modulus which are structural parameters.

Type 316 stainless steel have been investigated extensively in our laboratory by using our state variable approach (6,7). Because of its high melting temperature and impurity content, the dislocation structure developed at room temperature is highly stable. It is of interest also because of its low stacking fault energy ($\sim 20 \text{ erg/cm}^2$). Its dislocations are extended resulting in planar deformation behavior.

Experiments:

The dislocation structure examined was produced by uniaxial deformation in tension at a constant displacement rate of 0.02 inch/min. The specimen used had a gage length of one inch and a gage diameter of 0.113 inch. After reaching the desired plastic strain level in tensile loading, a load relaxation test was performed to determine the materials parameters of interest. The specimen was unloaded. Discs required for electron microscopy were prepared by spark cutting normal to the gage length.

The specimens for transmission electron microscopy (TEM) were prepared by mechanical polishing followed by electrochemical

thinning with a solution of methanol and nitric acid (2:1) at -50°C . A JEOL model 100B transmission electron microscope with a double tilting stage ($\pm 60^{\circ}$, $\pm 30^{\circ}$) was used for microstructural examination.

Results and Discussion:

The representative microstructure of solution treated type 316 SS specimen (vacuum annealed at 1200°C for 5 minutes then air cooled) prior to deformation is shown in Fig. 1 (magnification 25,000X). Figs. 2-5 show typical micrographs magnification 25,000X obtained from specimens deformed into the microplastic region and at 2%, 5% and 8% plastic strain respectively.

It is seen from these micrographs that increased non-elastic deformation results in the formation of low angle grain boundaries on activated slip planes with decreased spacing (d) between them. Figs. 3-5 were obtained by tilting the specimen so that the low angle grain boundaries are parallel to the electron beam in order to reveal the spacing (d) between them.

The dislocation structure of the low angle grain boundary can be observed by tilting the boundary normal to the electron beam as shown in Fig. 6 ($\sim 3\%$ plastic strain). The plane of the boundary was determined to be (111) type with dislocations of the type $1/2 \langle 110 \rangle$ having a mixed character in the order of 30° from the screw orientation.

For each plastic strain level, more than 200 spacings were evaluated to determine the mean spacing (d) between neighboring activated slip planes. The value of the hardness parameter σ_1^*

was also determined for each plastic strain level by the load relaxation test. Figs. 7 and 8 show a plot of spacing (d) vs. plastic strain level and vs the hardness parameter σ_1^* respectively. It is seen from these two figures that well defined correlations can be established among these variables. We are in the process of examining the physical significance of these correlations.

The stability of the dislocation structure was investigated by annealing the specimen in situ at elevated temperatures. Figs. 9 and 10 show the dislocation structure ($\sim 4\%$ plastic strain) before and after annealing the thin foil in situ at 500°C for approximately 2 hours by using a heating stage. It is seen that only minor dislocation rearrangement occurred while the main feature of the structure remain unchanged.

The formation of low angle grain boundary on well defined activated slip planes is a result of the planar deformation behavior of extended dislocations. Similar net work of low angle boundaries of type $a/2 \langle 111 \rangle$ dislocations has been observed in other fcc materials (8,9). A knitting mechanism has been proposed for the formation of the low angle boundary which is given in detail in reference 9.

In our second generation deformation model (10,11), as mentioned previously, we assume the existence of barriers to dislocation motion of varied strength. Plastic deformation is controlled by dislocation motion overcoming the

strong barriers which are characterized by a hardness parameter σ_1^* . Between neighboring strong barriers there is a distribution of weak barriers of varied strength which governs microplastic deformation and is characterized by another hardness parameter σ_2^* . Since microplastic deformation is produced by dislocation motion between strong barriers, the microplastic modulus M_1 is related to mobile dislocation density and the spacing between neighboring strong barriers. Anelastic deformation is produced by dislocation motion between two neighboring weak barriers which is time dependent and recoverable (12). The anelastic modulus M_2 is therefore related to the mobile dislocation density and spacing between neighboring weak barriers.

The parameters described above are all the structure related ones. The other parameters of the deformation model are concerned with the rate of dislocation motion. We have been able to identify features of the dislocation structure directly corresponding to all the structure related parameters.

The micrograph shown in Fig. 11 can be used to illustrate the relation between dislocation structure and structure related parameters. The micrograph shows typical dislocation structure produced by plastic deformation to about 5%. The strong dark lines in the micrograph represent well developed low angle grain boundaries on activated slip planes. The weak and less continuous lines are not fully developed low angle grain boundaries. We have identified the strong lines with strong barriers to dislocation motion and the weak lines with weak barriers. Since the

spacing between neighboring strong barriers and that between neighboring weak barriers have been found to be proportional to each other, we have taken the spacing between neighboring activated planes to be a measure of the hardness parameter σ_1^* which governs plastic deformation as shown in Figs. 7 and 8. We are in the process of evaluating dislocation density of less developed boundaries, based on the dislocation length or area of activated slip plane for relations with the hardness parameter σ_2^* which governs microplastic deformation.

According to the physical basis of the second generation deformation model, the ratio of microplastic modulus M_1 and anelastic M_2 should be inversely proportional to the ratio of spacing between neighboring strong barriers and that between neighboring weak barriers. The value of the latter ratio obtained based on micrographs such as the one shown in Fig. 11 has been found to be consistent with our recent measurement of the ratio of moduli (10, 11, 12).

We feel that we have made an important step forward during the past year in the development of the structural basis for our deformation models. We shall continue work in this direction as well as in the direction to develop dislocation structure based theories.

GRAIN BOUNDARY ANELASTICITY AND GRAIN BOUNDARY SLIDING

In this section we shall report work in this area on model development and on load relaxation tests. At the present we are in the process of using the experimental data obtained to determine the level of complexity required to model the phenomena of grain boundary anelasticity and grain boundary sliding. We are taking the same approach as the one which we have adopted in our work on grain matrix deformation that is, we are interested to construct phenomenological models which use the least number of materials parameters. We also require that the parameters used be evaluated experimentally.

Computer Simulation:

As reported in the previous progress report that we have proposed phenomenological models of increasing complexity which are capable of describing both grain boundary anelasticity and grain boundary sliding in a unified manner. A schematic representation of the model which contains the most number of components is shown in Fig. 12. In our model development we have used the approach originally proposed by Hart to combine the grain matrix deformation and grain boundary sliding in parallel (13). As shown in Fig. 12, the upper branch of the model includes an elastic element and a grain matrix element. The grain matrix element contains the three components of Hart's original model. The lower branch includes an elastic element, a grain matrix element and a

grain boundary element. The grain boundary element contains also three components equivalent to those of the grain matrix element. The physical significance of this model was discussed in the previous progress report (12). The constraint equations and the constitutive equations required for the model shown in Fig. 12, are given in Table I. It is seen from this table that a large number of equations are involved and the flow equation for the plastic elements ($\dot{\alpha}_I$, $\dot{\alpha}_{II}$ and $\dot{\alpha}_g$) are known to cause convergence problems. As expected, we have encountered numerical problems in computer programming. During the past year we have developed a simulation program based on the above model. The computer program with appropriately chosen parameters (Table II) has been used to simulate successfully the load relaxation data of Type 316 stainless steel which show the effects of grain boundary sliding (7). The simulation results are shown as the solid line in Fig. 13. The computer program can be used also to simulate a closed stress-strain loop obtained in a tensile test at a constant extension rate in the anelastic region (Fig. 14). As discussed in the previous progress report, when grain boundary effects are important, the lower portion of the data of a closed stress-strain loop obtained in loading measures grain matrix anelasticity. The upper portion of the loading data will contain both grain boundary and grain matrix anelastic effects.

We do not consider that our work is complete based on our success described above by using fitted parameters in computer simulation. We feel that with a sufficient number of parameters

one can always simulate deformation data of interest. We prefer to determine the required parameters, if possible, from independent experiments. Efforts made in the latter direction will be reported next.

Experiments:

We have chosen polycrystalline nickel to be the first material for which we shall develop the required experimental data to characterize grain boundary anelasticity and grain boundary sliding. The specimens used were Nickel 270 and have a grain size of 70 μm . As discussed in our previous progress report we shall use the closed stress-strain loop obtained by loading and unloading in a constant extension rate tensile test to provide information on grain boundary anelasticity. We shall perform load relaxation tests in the plastic deformation region to measure the contribution of grain boundary sliding. If the load relaxation data obtained are in the form of an S-shaped curve in a logarithmic stress vs. logarithmic non-elastic strain rate plot, we shall be able to obtain quantitative information on stress concentration produced by grain boundary sliding as well as on the flow behavior of the grain boundary. We plan to perform load relaxation tests also in the anelastic region to produce additional experimental information.

The phenomenological model shown in Fig. 12 as discussed in our previous progress report, can be simplified to contain a grain boundary element consisting of a single flow component as shown in Fig. 15. Based on our experimental data we are presently

in the process of determining if the simplified model will be adequate to describe both phenomena of interest in a unified manner.

We have obtained load relaxation data on Type 316 stainless steel in the form of an S-shaped curve (3,7). But similar data on pure metals such as lead (14) and aluminum (15) did not show the required S-shape. We believe that a metal of higher strength will have a better chance to exhibit the desired load relaxation behavior. We are extremely pleased that polycrystalline nickel did produce load relaxation data in the form of S-shaped curves.

Typical load relaxation data of polycrystalline nickel are shown in Fig. 16 (filled circular points). The open triangular points were obtained also in a load relaxation run performed after the previous run (filled points) by reloading the specimen to a stress level in the transient region. The significance of the reloading experiment was discussed in reference 16. The fact that the two sets of load relaxation data merge at low strain rates can be used to show that thermally induced structural changes are not important during the period of the experiment. The load relaxation data represented by the filled points were obtained at a total strain of about 3%.

The limiting behavior of the load relaxation data on both the high strain rate and low strain rate ends of the S-shaped curve can be used to determine the parameter Y of the constraint equation for the applied stress (Table I), the parameter Y measures the extent of stress concentration (7,13). The load relaxation data in Fig. 16 yield a value of Y approximately 0.84.

The value of Y can also be determined from the closed stress-strain loop, as discussed in our previous progress report if the simplified model is applicable. A representative closed stress-strain loop reported previously is reproduced in Fig. 17 which is obtained from a specimen different from the one from which the load relaxation data were obtained. The specimen for the stress-strain loop had also a grain size of 70μ but has undergone a different thermal-mechanical history. According to our previous progress report the loop data yielded a value of Y approximately 0.89.

We are in the process of assessing if the two values of Y are sufficiently close to justify the applicability of the simplified model. If it is not we shall have to rely on the model given in Fig. 12 for our interest. We are also in the process to obtain both the loop data and the load relaxation data from the same specimen in order that we can test further the validity of these alternate models.

GRAIN CAVITATION PROCESS IN THE ZIRCALOYS

Grain boundary cavitation during creep is closely related to grain boundary sliding. In a previous work we have investigated the effects of redistribution of the component of the applied stress normal to the grain boundary on the kinetics of cavity growth (17). The stress redistribution is produced by grain boundary sliding such that the magnitude of the stress component normal to the grain boundary is reduced. Stress normal to the grain boundary is the driving force for cavity growth for conditions where stress induced mass transport is the predominant mechanism.

As described previously, grain boundary sliding will influence also the nucleation of creep cavities. Cavity nucleation during creep has been shown to result from tensile stress concentration at grain boundary corners, steps and second phase particles in the grain boundary (18). The magnitude of the stress concentration is related to the geometry involved as well as the extent of flow incompatibility at these sites which is proportional to the displacement produced by grain boundary sliding.

One can easily visualize that at low creep strains sufficient stress concentration will be produced at sites where flow incompatibility is favored such that early nucleation will occur there. For sites where deformation incompatibility is not favored, large creep strain will be required prior to cavity nucleation. Phenomena such as grain boundary migration and recrystallization, which may relieve stress concentration produced by deformation

incompatibility, will prolong the incubation time for cavity nucleation and reduce its rate. As mentioned previously the contribution of grain boundary sliding will not be a simple function of temperature such that we do not expect that the kinetics of creep cavity nucleation will vary with temperature in a monotonic fashion.

Experimental results have been reported in the literature which can be used to support the physical picture described above. For example, the number density of creep cavities have been found to be related to creep strain which contains the contribution of grain boundary sliding (18). It should be recognized that current theories for the rate of nucleation and for the incubation time for phase transformation in the condensed systems are developed primarily based on clustering reactions. Because of the deformation incompatibility required to generate stress concentration for cavity nucleation, we do not expect that these theories can be applied directly for the present interest. We are in the process of formulating the required models for the incubation time and for the rate of cavity nucleation.

The results of the experimental effort on creep cavity nucleation are shown in Figs. 18-20. In these figures, the creep strain and the number density of cavities are plotted as a function of time. It is seen that correlations between creep strain and the number density of cavities exist for the data obtained at two lower temperatures. At 400°C where grain boundary migration, recovery and recrystallization are expected to occur, the correlation between these two variables is less obvious based on the data

shown in Fig. 20. We are continuing our experimental effort. We plan to generate cavity nucleation data covering a sufficient range of experimental conditions so that we can develop a required data base for model development. It is interesting to note that in literature there are far more theoretical papers on nucleation than experimental ones.

MATERIALS CHARACTERIZATION BY USING THE STATE VARIABLE APPROACH

During the past year we have used our state variable approach to investigate the effects of texture on the deformation properties of several Zircalloys in a joint project with EPRI. We have been able to use load relaxation tests to obtain information on grain boundary sliding and flow properties of these materials which are not easily obtained by using traditional testing methods. Knowledge of these properties are useful for the purpose of optimizing the cladding behavior of Light Water Reactor (LWR) fuel pins.

The results of our work on the Zircalloys are included in a report for publication (see list in the Introduction section). The capabilities of the load relaxation test to reveal flow properties as influenced by texture can be illustrated by using the data shown in Figs. 21 and 22. These data were obtained under approximately the same conditions with tensile specimens fabricated from Zircaloy sheets. For the 0° textured specimen the basal pole is normal to the plane of the sheet. The difference in flow behavior between the 0° and 30° textured specimens can be easily seen from the shape and the position of the curves in these figures. A detailed discussion of the significance of these data is given in the report on this work.

We have developed also constitutive equations which describe the deformation properties of 20% cold worked Type 316 stainless steel in a joint effort with HEDL. These constitutive equations as mentioned previously include the effects of simultaneous

recrystallization during deformation. We have been able to use these equations together with our stress analysis code for internally pressurized thin walled tubes to simulate the behavior of these tubes under a variety of loading conditions. Typical results of our simulation calculations are shown in Figs. 23-25. A detailed discussion of this work is included in two reports listed in the Introduction section.

It should be noted that the data shown in Figs. 23-25 involve three different loading modes, and time scales differing by several orders of magnitude. The materials parameters of the constitutive equations were evaluated based on our experimental data (6,7) and HEDL data obtained by using traditional testing methods. The success of our simulation is encouraging and demonstrates the need for our participation directly in the application of our findings.

RESEARCH IN MECHANICS

An important goal of the work in mechanics is to develop efficient computational techniques for the analysis of deformation of structures with material behavior governed by our state variable models. These capabilities are of crucial practical importance for the design of structural components subjected to stresses at elevated temperatures. We are also in the process of investigating phenomena of materials interest such as fracture by taking advantage of the same computational capabilities.

The analytical research performed during this period has continued the applications and refinements of the Boundary Element Method (BEM) and the Finite Element Method (FEM) to problems of time-dependent inelastic deformation of structures. A finite element program for the analysis of planar and axisymmetric problems using the state variable constitutive model had been developed during a previous contract period. In this period, this program was extended to include the effect of transient thermal stresses (19). Stress analysis in structural components subjected to time-varying thermal loads (in addition to mechanical loads) is of great importance in energy systems. The computer program is operational and has been applied to several sample problems.

Application of the boundary element method to problems of time-dependent inelastic deformation of thin plates started during the last contract period, has been concluded during this period (20). The resulting computer program can be used to predict stresses and

deformations in thin plates of arbitrary shape with clamped or simply supported boundary conditions. Sample results predict the proper pattern of time-dependent deformation of plates as well as redistribution of stress through the plate thickness anywhere in the plate. The stress distribution through the thickness changes from the initial elastic distribution to an elastic-plastic one. Once again, the state variable constitutive model has been used here to describe the plate material.

The major thrust of the applications of the boundary element method, during this contract period, has been in the area of time-dependent inelastic fracture mechanics (21-24). While the boundary element method had been previously demonstrated to be very effective for the analysis of deformation of bodies of regular shape, it appeared to have limitations if the body in question had a sharp cutout or crack present in it. This difficulty arises because the discretization of a crack surface requires a very large number of boundary elements on it in order to accurately determine the large stresses near a crack tip. This can lead to numerical ill-conditioning. A novel approach has been developed during this contract period that overcomes this difficulty in an elegant manner. This approach involves the augmentation of the previous kernels so that the new kernels are the singular solutions for infinite regions with a crack already present in it. Use of these kernels guarantees the satisfaction of proper boundary conditions on the crack surface in an implicit manner. Thus, discretization of the crack boundary is no longer necessary in a

numerical solution procedure. The solution procedure using this method is very efficient. Numerical results for cracked plates under inplane tension and shear loading (Mode I and II) and anti-plane shear loading (Mode III) are presented in references (21-23).

A complete analytical solution for the problems solved numerically in references 21-23 do not exist. However, asymptotic analytical solutions have been recently obtained by other researchers for line cracks in infinite plates obeying an elastic-power law creep constitutive model. Comparison of the boundary element method solutions with these asymptotic solutions is currently in progress (24) and a report describing these results will be completed during the period September-November 1980.

A start has been made in the study of void growth, in bodies undergoing inelastic deformation governed by the state variable constitutive model. A void is considered spherical and a computer program for the analysis of problems with spherical symmetry, developed some years ago, is ideally suited for the problem. The growth of a spherical void under internal pressure and the redistribution of stresses with time near the void is being studied using the realistic constitutive model for material behavior. A report with initial results will be completed during the next three months.

Some details of the research performed in this program, during the current period, follow.

Finite Element Program:

A finite element method computer program for time-dependent inelastic analysis of structures, developed during a previous contract period, has been extended to include the effect of thermal transients (19). This program can now be used to solve plane stress, plane strain and axisymmetric problems. Material behavior is governed by the state variable constitutive model and time-varying temperature fields and associated thermal stresses are included in the program. The temperature field is determined by solving the appropriate diffusion equation. Either the quasi-steady or the unsteady diffusion equation option could be used.

Fig. 26 compares results from the finite element program with direct solutions for a sample problem of a uniform thick cylinder in plane strain, whose inside surface is heated at a constant rate. The FEM solution is seen to agree very well with a direct solution. As expected, the quasi-steady and unsteady FEM results coincide for a low heating rate (7.2°C/hr where thermal transient effects are not important) but differ substantially for a rapid heating rate (5.6°C/sec). The latter heating rate is that being used by national laboratories to simulate loss of coolant transients in nuclear reactors.

A problem of practical interest is the determination of the effect of grooves in a gas cooled fast breeder reactor (GCFR) fuel element cladding on the stress and deformation distribution. These grooves are cut into the tube to improve heat transfer between the tube and its surroundings. Using representative dimensions

from Argonne National Laboratory, a portion of the GCFR tube is shown in Fig. 27. The finite element discretization is shown in the same figure. The inside radial displacement at a point in the tube is shown as a function of time in Fig. 28. The loading is purely thermal and the temperature throughout the tube is assumed to increase uniformly at 5.6°C/S . This represents a loss of coolant transient. The displacement in Fig. 28 is seen to increase with temperature. The initial displacement of about 0.417 mil is elastic, and this is followed by anelastic, thermal and permanent deformation. The anelastic deformation, which is partially recoverable upon unloading, is obtained from the deformation of the anelastic spring in the constitutive model, while the permanent deformation, from the 'plastic' element is irrecoverable.

Plate Bending by the Boundary Element Method:

Structural components, which have one dimension smaller relative to the other two, are often modelled as thin plates. The study of transverse deformation of thin plates of arbitrary shape is an important subject in mechanics. An analysis of inelastic transverse deflection of thin plates of arbitrary shape, by the boundary element method, has been completed (20). Once again, the nonelastic deformation of the plate is described by the state variable constitutive model. The computer program can be used to solve problems for clamped or simply supported plates subjected to arbitrary time-varying transverse loads. Thus, realistic time-histories of loads, important to the design of

structural components (in nuclear reactors for example), can be input into the computer program.

Fig. 23 shows the variation of central displacement of a clamped square plate as a function of applied load. The load is uniform in space and is assumed to increase at a constant rate. The elastic, anelastic and permanent deformations are evident in the figure. The change in the stress distribution through the plate thickness, from the linear elastic to the nonelastic, is shown in Fig. 30. The constitutive model used does not have an explicit yield surface. It can, nevertheless, predict yield like phenomena as in a plasticity model. In this context yielding means the transition into the viscoplastic limit region of the constitutive model. This is the region where the anelastic stress approaches the hardness in the 'plastic' element, thereby causing substantial permanent deformation. Yielding, in this problem, starts at the midpoints of the outside edges of the plate. The yield front starts moving out along the plate edges and then a second yielding occurs at the center of the plate (21). These phenomena are in general agreement with plasticity model but, of course, the state variable model is much more general.

Inelastic Fracture Mechanics by the Boundary Element Method

A major advance has been made in the applicability of the boundary element method during the current period. This advance is the efficient use of the BEM for the calculation of stresses in cracked bodies undergoing time-dependent inelastic deformation. This new development has been made possible by the use of modified

kernels in the integral equations. These kernels satisfy the appropriate boundary conditions on a crack surface in an implicit manner so that discretization of the crack boundary is no longer necessary in a numerical solution procedure. Thus possible ill-conditioning which might result from such a discretization, is avoided.

A computer program has been developed using this idea. This program can be used to analyze stresses in cracked planar bodies of arbitrary shape subjected to in-plane tension or shear (Mode I or II) (22,23) or anti-plane shear loading (Mode III) (24). The loads can vary in time in an arbitrary fashion. A crack is modelled as a very thin elliptical cutout and the plate material can be described either by a conventional (e.g. power law creep) or state variable type constitutive model.

Numerical results for some sample problems are shown in Figs. 31-33 (Mode I) and 34,35 (Mode III). The stress concentration at the tip of a stationary crack, as a function of time, for tensile loading increasing at a constant rate, is shown in Fig. 31 (power law creep) and 32 (state variable model). The decrease of stress concentration with time is due to flow of the material in the high stress region near the crack tip, and consequent accommodation of stress. The time-scales of the results from the two models (Figs. 31 and 32) are different because the state variable constitutive model simulates short time transient as well as steady state response. The results in Fig. 32 are for transient response for short times. The 'bumps' in Fig. 32

require further investigation. They may be due to numerical problems.

The growth of the viscoplastic region near a crack tip, using the state variable model, is shown in Fig. 33. The area inside the region, at any given time, is where substantial permanent deformation takes place. As expected, the viscoplastic region starts at the crack tip and grows with time.

Similar results for anti-plane shear loading (Mode III) is shown in Figs. 34,35. This time the remote loading is constant and the power law creep constitutive model is used to describe material behavior. The stress near the crack tip is seen to redistribute rapidly with time (Fig. 35). The flow of the material causes the stress to even out with time.

A complete analytical solution for those problems do not exist. Comparisons of these solutions are currently in progress with asymptotic solutions obtained by other researchers. These asymptotic solutions are for line cracks in infinite plates described by an elastic-power law creep constitutive model. They are obtained by neglecting the elastic strain rates relative to the nonelastic ones near the crack tips. A report describing these comparisons will be ready soon.

TABLE I

CONSTITUTIVE EQUATIONS FOR GRAIN BOUNDARY DEFORMATION

(Fig. 12 Full Model)

Constraint Equations

$$\sigma = Y\sigma_I + (1-Y)\sigma_{II}$$

$$\sigma_I = \sigma_{aI} + \sigma_{fI}$$

$$\sigma_{II} = \sigma_{aII} + \sigma_{fII}$$

$$\sigma_{II} = \sigma_{ag} + \sigma_{fg}$$

$$\dot{\epsilon} = \dot{\epsilon}_I + \dot{\epsilon}_{II}$$

$$\dot{\epsilon} = \dot{\epsilon}_{II} + \dot{\epsilon}_{II} + \dot{\epsilon}_g$$

$$\dot{\epsilon}_I = \dot{a}_I + \dot{\alpha}_I$$

$$\dot{\epsilon}_{II} = \dot{a}_{II} + \dot{\alpha}_{II}$$

$$\dot{\epsilon}_g = \dot{a}_g + \dot{\alpha}_g$$

Constitutive Relations

$$\sigma_I = Ee_I$$

$$\sigma_{II} = Ee_{II}$$

$$\sigma_{aI} = M_{aI}$$

$$\sigma_{aII} = M_{aII}$$

$$\sigma_{fI} = (\dot{\epsilon}_I/K)^{1/M}$$

$$\sigma_{fII} = (\dot{\epsilon}_{II}/K)^{1/M}$$

$$\ln(\sigma^*/\sigma_{aI}) = (\dot{\epsilon}^*/\dot{\alpha}_I)^\lambda$$

$$\ln(\sigma^*/\sigma_{aII}) = (\dot{\epsilon}^*/\dot{\alpha}_{II})^\lambda$$

$$\sigma_{ag} = M_{ag}$$

$$\sigma_{fg} = \dot{\epsilon}_g/k_g$$

$$\ln(\sigma_g^*/\sigma_{ag}) = (\dot{\epsilon}_g^*/\dot{\alpha}_g)^\lambda$$

$$\dot{\sigma}^* = \sigma^* \Gamma \dot{\alpha}_I$$

$$\dot{\epsilon}^* = D(\sigma^*)^m$$

TABLE II

PARAMETERS USED TO SIMULATE GRAIN BOUNDARY SLIDING

(Solid S-shaped curve in Fig. 13)

Young's Modulus = 30×10^6 psi.Machine Compliance = 3×10^{-5} (1/psi.)

Initial Length = 1 in.

Initial Area = 0.785×10^{-2} in²Lambda (λ) = 0.15

Capital M = 7.6

Small m = 4.5

Dislocation Glide Constant (K) = 0.15×10^{-18} Initial Sigma Star ($\sigma_{\text{initial}}^*$) = 48230 psi.Initial Epsilon Dot Star ($\dot{\epsilon}_{\text{initial}}^*$) = 0.7986×10^{-3}

Stress Concentration factor (Y) = 0.838

Beta (β) = 0.17×10^6 Delta (δ) = 1.33Script MG (M_g) = 0.3×10^9 psiGrain Boundary Friction Factor (Kg) = 0.1×10^{-9} Grain Boundary Sigma Star (σ_g^*) = 0.11×10^6 Grain Boundary Epsilon Dot Star ($\dot{\epsilon}_g^*$) = 0.1×10^{-5} Grain Boundary Lambda (λ_g) = 0.32Initial $\sigma_{aI} = 0$ Initial $\sigma_{aII} = 0$ Initial $\sigma_{ag} = 0$ Initial Stress $\sigma = 10$ psiSigma I (σ_I) = 11.89 psiSigma II (σ_{II}) = 0.22 psi

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FIGURE CAPTIONS

- Fig. 1. Microstructure of solution treated type 316 SS observed by transmission electron microscopy, magnification 25000X.
- Fig. 2. Microstructure of type 316 SS after deformation into the microplastic region showing dislocation pile-ups against grain boundaries (25000X).
- Fig. 3. Microstructure of type 316 SS after deformation, 2% plastic strain, showing the formation of low angle grain boundaries on activated slip planes (25000X).
- Fig. 4. Microstructure of type 316 SS after deformation, 5% plastic strain, showing the formation of low angle grain boundaries on activated slip planes (25000X).
- Fig. 5. Microstructure of type 316 SS after deformation, 8% plastic strain, showing the formation of low angle grain boundaries on activated slip planes (25000X).
- Fig. 6. Microstructure of type 316 SS after deformation, 3% plastic strain, the specimen is tilted so that the electron beam is perpendicular to the low angle grain boundaries showing the dislocation structure of the low angle grain boundaries on the activated slip planes (25000X).
- Fig. 7. Plot of the spacing (d) between the activated slip planes vs. the accumulated plastic strain.

- Fig. 8. Plot of the spacing (d) between the activated slip planes vs. the hardness parameter σ^* .
- Fig. 9. The dislocation microstructure of a selected area showing individual dislocations for type 316 SS deformed to 4% plastic strain (25,000X).
- Fig. 10. The same region as in Fig. 9 after annealing in situ at 500°C for 2 hours showing that the main features of the dislocation microstructure remain unchanged (25,000X).
- Fig. 11. Microstructure of type 316 SS after 5% deformation, showing the existence of less developed low angle grain boundaries between the fully developed low angle grain boundaries (25,000X).
- Fig. 12. A schematic representation of the phenomenological model for grain boundary deformation (full model).
- Fig. 13. Load relaxation data (solid dots) for type 316 SS at 600°C in the plastic range showing the effect of grain boundary sliding (S-shaped curve). The two dashed curves represent two limiting grain matrix controlled relaxation behavior, the solid (S-shaped curve) is simulated by using the phenomenological model for grain boundary sliding (Fig. 12).
- Fig. 14. Stress-strain loop obtained by simulation by using the phenomenological model for grain boundary sliding (Fig. 12).

Fig. 15. A schematic representation of the simplified model for grain boundary sliding.

Fig. 16. Load relaxation data for Nickel 270 at 600°C showing the effect of grain boundary sliding (S-shaped curve, filled dots). The specimen is unloaded then reloaded to a lower stress level (open triangular points) showing microstructural stability during the load relaxation run.

Fig. 17. Stress-strain closed loop for Nickel 270 at 600°C obtained in a constant extension rate tensile test by loading and unloading in the anelastic range.

Fig. 18. Measured number density of creep cavities in Zircaloy-2 at 350°C in the same plot with the creep strain of the specimen.

Fig. 19. Measured number density of creep cavities in Zircaloy-2 at 375°C in the same plot with the creep strain of the specimen.

Fig. 20. Measured number density of creep cavities in Zircaloy-2 at 400°C in the same plot with the creep strain of the specimen.

Fig. 21. Load relaxation data at 350°C for Zircaloy-4 (9913-3B) $\pm 30^{\circ}$ textured at several strain levels.

Fig. 22. Load relaxation data at 350°C for Zircaloy-4 (9913-4B) 0° textured at several strain levels.

Fig. 23. Experimental data (lines) and simulated results (dots) for thin walled 316 SS thin walled tubes for the temperature transient mode at different internal pressures for the case $\dot{T} = 5.6^{\circ}\text{C/sec}$.

Fig. 24. Experimental data (dots) and simulated results (dashed and solid lines) for creep of 316 SS thin walled tubes at 650°C and different internal pressures.

Fig. 25. Experimental data (dots) and simulated results (solid line) for the constant circumferential displacement rate mode for 316 SS thin walled tubes at 425°C .

Fig. 26. Inside circumferential strain as a function of inside temperature for an uniform thick cylinder in plane strain. $b/a = 1.5$, $T_a(0) = 100^{\circ}\text{C}$, $T_b = 100^{\circ}\text{C}$, $\sigma_o^* = 17 \text{ ksi}$.

Fig. 27. Finite element mesh for GCFR tube in plane strain. Dimensions in inches.

Fig. 28. Inside radial displacement at $z = 0$ in a GCFR tube in plane strain as a function of temperature. Internal pressure = 10 ksi, $T(r,z,0) = 25^{\circ}\text{C}$, $\dot{T}(r,z,0) = 5.6^{\circ}\text{C/s}$, FEM-quasi-steady. $\sigma_o^* = 95 \text{ ksi}$ (cold worked specimen).

Fig. 29. Load as a function of central displacement for a clamped square plate subjected to a uniform load increasing at a constant rate.

Fig. 30. Redistribution of stress at the mid-point of an edge of the clamped square plate of Fig.24.

Fig. 31. Stress concentration at crack tip as function of time. Mode one. Power law creep model.

Fig. 32. Stress concentration at crack tip as function of time. Mode one. State variable model.

Fig. 33. Growth of viscoplastic region in cracked plate. Mode one. State variable model. $\dot{\sigma}_{22}^{\infty} = 244$ psi/sec.

Fig. 34. Stress concentration at crack tip as a function of time for constant remote stress. Mode three. $\sigma_{32}^{\infty} = 1000$ psi, $a/b = 199$. Initial stress concentration = 204. Power law creep.

Fig. 35. Stress redistribution along the line $x_2 = 0$ in cracked plate for constant remote stress. Mode three $\sigma_{32}^{\infty} = 1000$ psi, $a/b = 199$. Power law creep.

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