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3D Computations and Experiments

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3D Computations and Experiments

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This project is in its first full year after the combining of two previously funded projects: *3D Code Development* and *Dynamic Material Properties*. The motivation behind this move was to emphasize and strengthen the ties between the experimental work and the computational model development in the materials area. The next year's activities will indicate the merging of the two efforts. The current activity is structured in two tasks. Task A, *Simulations and Measurements*, combines all the material model development and associated numerical work with the materials-oriented experimental activities. Task B, *ALE3D Development*, is a continuation of the non-materials related activities from the previous project.

Task A: Simulations and Measurements (1000K)

Technical Problem

The understanding of material properties and the ability to produce accurate representations of those properties in numerical simulations of dynamic events is of great importance to the development and fielding of weapon systems. Examples where material properties play a critical role include explosively formed penetrators, long rod penetrators, shaped charges, penetration mechanics, fracture and fragmentation. The physical phenomena that determine material properties and material response to loading and deformation can be quite complex. Often a physical understanding of macroscopic response can only be understood in terms of models for the microscopic properties and response.

The goal of this project is to develop physically-based models of the 3D response of materials to dynamic loading that can be utilized in simulation codes to address the applications listed above. The focus will be on attaining a predictive capability for the evolution of constitutive response and for the initiation and evolution of fracture. The project will combine experimentation and model development activities. The experiments will be designed to evaluate microscopic properties and response in order to provide the data and knowledge required to construct macroscopic models for use in continuum level simulation codes.

Expected Payoffs

The understanding and potential control of material properties that can arise from the multiscale model approach allows one to envisage significant advances in the technology associated with the manufacture of metal components. Many characteristics of metal parts are directly related to attributes that can only be understood by characterizing the properties of the utilized material at the meso- and micro-scales. If one could translate such knowledge into models that would both represent and evolve those properties through a forming process, then one would have attained a greater degree of control of the attributes that determine the performance of the formed part in its intended application. The manufacture of liners and the dynamic formation of shaped charge jets and explosively formed projectiles are the most ready examples of relevant applications. The same physical considerations can be applied to the potential for understanding and control of fracture and fragmentation.

Technical Status and Issues

A combined experimental and computational approach is required to produce models with predictive capability. The model development activity has focused on the representation of anisotropic material response, improved representations of constitutive properties at high strain rates, and improved damage and failure models. The experimental work will focus on providing the data required to elucidate the basic physical mechanisms and to validate the derived models.

The multiscale modeling approach has demonstrated considerable promise for the development of models of material response. Information obtained from experimental and theoretical studies at the lower length scales is contributing to the formulation and utility of continuum level models. Continued research is required to bring these models to a state at which they can regularly contribute to design and development activities.

Summary of Current Year's Work

Model Development

Activities in this area include developing models to represent anisotropic material properties, an improved representation for constitutive properties at high strain rates, and improved material damage and failure models. This activity is part of a broader effort intending to incorporate the results of investigations at the atomic-, micro-, and meso-scale levels into continuum models for the above processes. This effort also supports continued development of a variety of macro-scale models for the ALE3D user community.

Progress has been made in the development of a formalism for treating anisotropic plasticity. The implementation in ALE3D has been extended to include dynamic evolution of the yield surface and rate dependent hardening. The physical models for determining the course of this evolution in yield surface are still under development. Some success has been attained in trying to predict the rotation observed in some shaped charge jets and attributed to anisotropic liner properties. The attempt has been made to start with measured microstructural features of a fabricated liner, produce an anisotropic response model from the observed properties, and then predict the observed rotation in a 3D calculation of the liner collapse and jet formation. Qualitative success has been attained in that jet rotation is observed. Continued work is needed to get better quantitative agreement with the amount of rotation.

Crystal plasticity modeling has been extended to allow for more accurate treatment of strong shocks. The goal of this meso-scale modeling is to shed light on the physical processes by which micro-structural features affect macro-response. Application areas include yield surface evolution under deformation, strain localization, and free surface effects.

Simulations of dynamic fracture experiments have produced results that indicate that a model representing the actual statistical distribution of damage initiation sites and their effect on local fracture response can be used to predict fragment characteristics such as fragment size distributions. This modeling activity suggested a series of experiments to test this hypothesis. This will be discussed further below.

Experiments

Recent activity has focused on formulating a new experimental test program that closely aligns with the theoretical and numerical model development efforts. To that end, the current plan is to retain support of one of the previous experimental efforts, the one referred to as the *polycrystal virtual test sample*. The remainder of the activity will focus on experiments aimed at supporting the development of physically based models of material fracture.

Planned Work

Model Development

Code development activities will continue to focus on providing enhanced capabilities in the areas of advanced material models. Activities in this area include developing models to represent anisotropic material properties, an improved representation for constitutive properties at high strain rates, and improved material damage and failure models. This activity is part of a broader effort intending to incorporate the results of investigations at the atomic-, micro-, and meso-scale levels into continuum models for the above processes. Particular emphasis will be placed on modeling the various case fracture and fragmentation experimental studies underway. Physically-based material failure models must be tied to subscale phenomena to be generally useful and predictive. The model development will utilize the data being made available by the experimental activities and will suggest the most useful experiments for its purposes.

Experiments

Polycrystal Virtual Test Sample

A novel experimental approach has been developed to examine the influence of microstructure on single crystal constitutive behavior of Ta through the use of two-dimensional virtual test samples (VTS-2d). The combined use of this sample geometry with single crystal plasticity data facilitates the development of micro-structurally sensitive strength models suitable for engineering calculations that include the effects of crystallographic texture and grain morphology. This provides a critical link between single crystal and continuum plasticity.

LLNL has machined and heat-treated polycrystalline flat sheet samples. The goal of the heat treatment is to produce a very course "2-D" structure with grains running essentially through the sheet. The original orientation of each grain in the test sample is determined using orientation imaging microscopy (OIM). This information is used to construct a 3-D finite element mesh of the test sample. The sample is then deformed in tension, and is subsequently characterized again using OIM to determine grain rotations. This information can then be compared directly to simulation results.

Figure 1 illustrates a calculation in which crystal lattice orientations were mapped directly onto a finite element grid. Preliminary simulations use 75mm grid, but plans are to use 25mm grid.

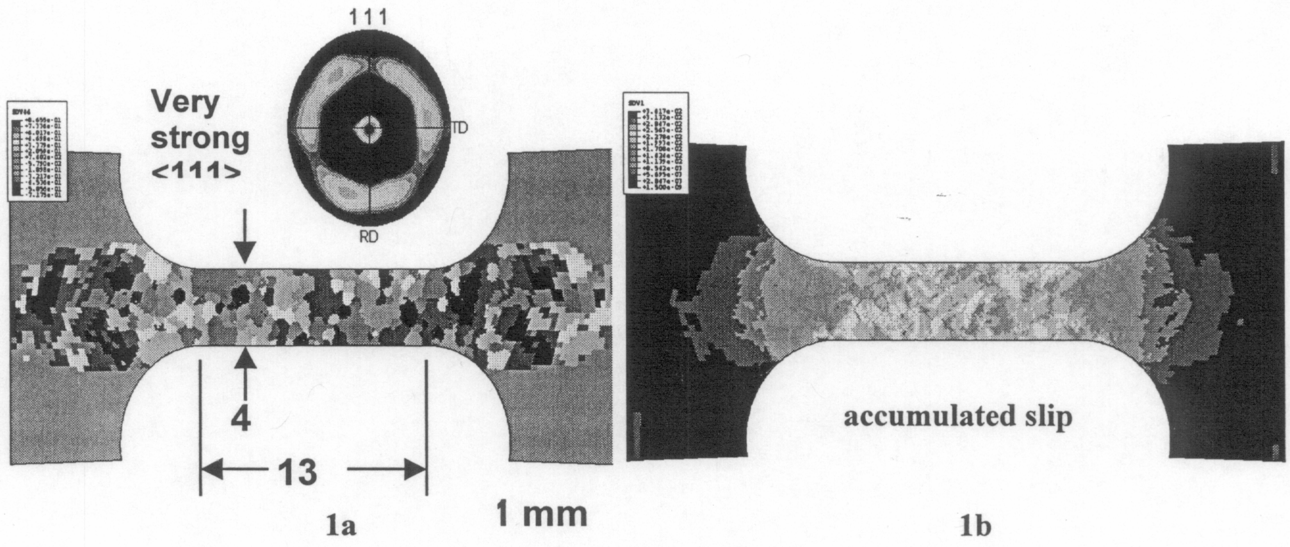


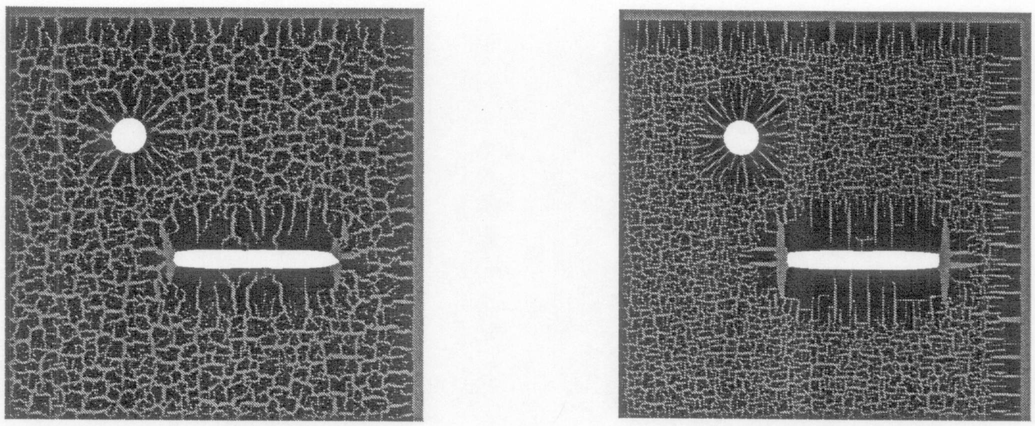
Figure 1: Crystal model validation simulation on columnar grain polycrystalline Ta tensile specimen. Figure 1a represents the crystal orientation data. Figure 1b presents the accumulated slip. The calculations were taken to 3.5% total slip.

A new specimen having a more truly columnar structure has been prepared. These experiments will be repeated and extended to larger strain at LLNL.

Fracture Experiments

A critical component of the multiscale modeling approach to fracture mechanics is the ability to predict the correlation between microstructure and fracture response. Ductile fracture is characterized by the nucleation, growth and coalescence of voids. During the nucleation and growth phases, a free-surface forms at *initiation sites* and grows under continued tensile loading. Subsequent void coalescence signifies a departure from a uniform to a localized strain-state and serves as a potential site for cascading material failure. Spatial and morphological distributions of initiation sites are evident in the microstructure of metals, suggesting that the coalescence phase may be accelerated in numerous, specific regions of a stressed body. Part of this investigation is to determine the role of spatial and morphological distributions of initiation sites in a material failure criterion. Under dynamic loading conditions, the formation of fragments is controlled in part by the local variations in fracture conditions.

The results of some numerical exercises have provided insight to an appropriate experimental approach. Figure 2 illustrates the results of simulations of a biaxially loaded plate with some assymetric features included. The calculation was performed using the Johnson-Cook model with allowance for a statistical variation in the local fracture strain. As indicated in Figure 2, the larger the dispersion in fracture strain the larger the produced fragments. A similar approach of using a statistical variation in failure strain was used to calculate an HE-driven cylinder. The qualitative comparison with experiment is illustrated in Figure 3.



e_0 = 0.3 +/- 0.05
larger fragments

e_0 = 0.3 +/- 0.01
smaller fragments

Figure 2. Simulations of a biaxially loaded plate. The calculation was performed using the Johnson-Cook model with allowance for a statistical variation in the local fracture strain. As indicated, the larger the dispersion in fracture strain the larger the produced fragments.

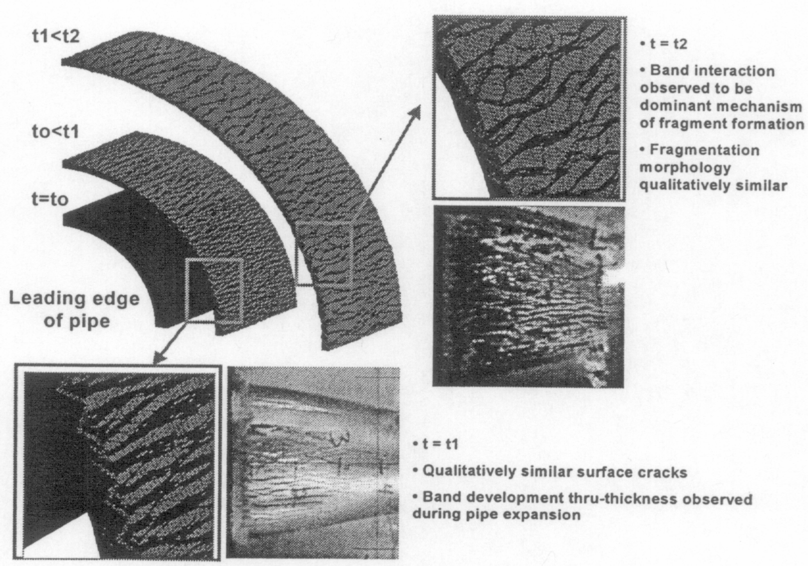


Figure 3: Simulations incorporating spatial and morphological distributions of initiation sites can be used to determine local failure condition variations that are qualitatively similar to experimental results

We have devised a formalism that will provide a characterization and testing process intended to provide this correlation. This activity is thus aimed at providing the basis for predictive model development and validation. The procedure that will be followed and evaluated includes:

- Perform quantitative metalography on pre-test material to characterize spatial and morphological distributions of the initiation sites in the microstructure
- Determine appropriate length-scale(s) using material characterization and testing
- Conduct suite of micro-scale, quasi-static experiments at determined length-scales to establish *statistically-significant* fracture strain variations
- Perform high strain rate experiments to provide validation data for model development (including in-situ diagnostics)
- Make relevant data accessible to microstructurally-based dynamic fracture model development and validation efforts

The materials being considered for this investigation are Aermet 100 for DoD applications and the aluminum alloy (AA 6061) because it is used in a variety of applications and possesses a microstructure conducive to studying initiation site distributions. This methodology can be readily applied to other materials to determine local fracture condition variations and appropriate length-scales.

WHA

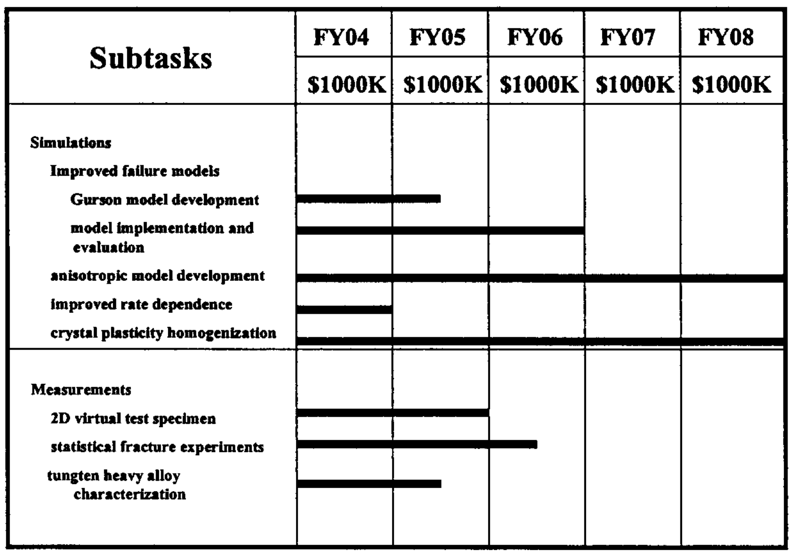
Metallurgical analyses and fractography are being performed on tungsten heavy alloy specimens provided by Army collaborators at ARL. The purpose is to gain further understanding of micro-structural properties in order to determine an approach to enhanced strength and ductility. Of interest are the evolution of properties through the fabrication process and the effect of these properties on fracture response.

Technology Transition

The modeling and experimental activities are communicated to DoD parties through the TCG process, by individual technical interchanges and by publication in the open literature. The material models being developed are generally resident in ALE3D, which is available to DoD facilities and contractors. These models are usually published in the open literature and can be made available as programmed routines for implementation in other simulation codes.

Milestones

Task A: Simulations and Measurements



Task B: ALE3D Development (600K)

Technical Problem

Accurate and efficient numerical simulations of hydrodynamic events are of great importance in munitions design and effectiveness activities. Computer simulations allow for rapid and detailed evaluation of warhead concepts at small incremental cost. As resource intensive experiments become less available, the cost effectiveness of numerical modeling will continue to increase.

Traditional hydrocodes are generally pure-Eulerian or pure-Lagrangian in format. The latter provide good geometric resolution, but their utility is severely diminished when large material distortions are encountered. Pure-Eulerian codes are capable of dealing with arbitrarily large material distortions, but satisfactory resolution often generates excessive memory requirements and calculation times. The arbitrary-Lagrange-Eulerian (ALE) format combines the resolution of a Lagrangian code with the capability of an Eulerian code to handle large distortions. LLNL has developed ALE techniques that provide a more efficient use of the computational mesh resulting in shorter calculations that require less computer memory.

ALE3D had its genesis with DYNA3D. The code has been completely rewritten and many of the algorithms have been altered or replaced, but the basic, finite element data structure has been maintained. The code currently treats only hexahedral solid elements, but the connectivity is allowed to be arbitrary in the sense that a single node can be shared with an arbitrary number of elements. This feature in itself leads to significant advantages in zoning efficiency over a regularly connected code like CALE. The grid can also be organized into independently zoned blocks that interact through slide surfaces. Intersecting slide surfaces are allowed as are the opening and closing of voids between blocks. A single-sided slide surface treatment allows the boundary of a block to fold back on itself. Calculations in Lagrangian regions can be performed with beam and shell elements. This capability, coupled with the ability to treat multifluid dynamics with an ALE mesh makes ALE3D a powerful tool.

ALE3D also provides a high level integration of a number of modeling options. Beam and shell elements are available to provide a more powerful structural representation. A version with heat conduction and thermal-chemistry has been developed. An implicit time integration scheme for the solution of the dynamics is also available for some applications. This software provides a unique aggregate of capabilities.

Expected Payoffs

The implementation of the ALE capability in ALE3D provides distinct advantages to the defense community. The improved resolution available:

1. provides greater accuracy,

2. allows more detailed investigation of physical phenomena,

3. extends simulation capability to more classes of problems.

Shortened computation times and diminished memory requirements:

1. improve cost effectiveness in R&D activities,

2. allow numerical modeling capability to be more widely available.

The combined thermal-chemical-mechanical simulation capability allows:

1. treatment of more complex simulations than previously possible,

2. treatment of vulnerability and lethality issue at closer to a full system level.

The availability of structural elements within the 3D ALE code represents a dramatic improvement in capability and efficiency, and will be of direct assistance in a number of applications of importance to the defense community. The availability of fully coupled thermal-mechanical solutions with chemical reaction allows a number of new applications to be addressed in the areas of weapon system vulnerability and lethality.

Technical Status and Issues

Code development activities are currently focused on providing enhanced capabilities in the areas of

- multiphase flow
- blast loading of structures

The past year has also produced a significant increase in the level of activity in the area of multiphase flow. The programmatic interest has been driven by missile defense issues associated with possible collateral effects from an intercept, and by the need to simulate complex explosive mixtures.

We have developed an expanded effort focused on providing a more powerful capability to represent structural response to blast loading. A number of important applications require the coupling of a hydrodynamic event to a larger structure, which may itself undergo severe distortion, in order to assess that structure's response. ALE3D provides the capability to perform these calculations consistently within a single code. However, the complexity of the structure may be so great that it is more efficient and accurate to revert to a coupled code approach. The plan is to provide communication links that will allow ALE3D to exchange information with both DYNA3D and NIKE3D. NIKE3D could then be used to generate the initial stresses in a structure due to gravitational loading. ALE3D could read in the NIKE3D results to provide the correct initial conditions for the blast calculation. ALE3D would then simulate the blast and determine the loading and the near field structural deformation. The blast state and the loading conditions could then be transferred to DYNA3D for the global structural response calculation.

The planned budget represents an increase for work under this task. The intention is to use this increase in resources to support a more aggressive interaction between the ALE3D code development efforts and the interested DoD-related community.

Summary of Current Year's Work

Blast Loading of Structures

The ALE3D user community has indicated considerable interest in broadening the material models available to include better representations of geologic materials. A clay model has been used successfully in simulations associated with earthen dams. Options for including existing models for various forms of rock are being evaluated.

Multiphase Flow

This activity is focused on improving the capability to simulate a range of phenomena usually associated with weapon system effects or vulnerability. Particular focus is provided by interest in an ability to predict collateral effects from a missile defense intercept of a chemical or biological warhead. The initial activities include improved models for non-ideal gases, models incorporating liquid to vapor transitions, developing a surface tension model to better treat liquid interfaces, and a particulate transport model. This activity partly consists of providing new code features such as those described above, and partly of using existing features in new modes. Utilizing the missile intercept of a chemical warhead scenario, a traditional hydrodynamic calculation of the intercept using viscous fluids could be used to predict the energy and momentum imparted to the chemical agent. This information, coupled with some experimental data, would allow for the deduction of size and velocity distributions of the ejected material. Simulations containing aerodrag, viscous flow and surface tension would provide information on the final droplet size and its interaction with atmospheric effects. Improved models for the representation of aerodrag, aeroheating and surface tension have been implemented. It is now possible to model the effects of surface tension in mixed material elements.

A second focus area has been added in the past year: the simulation of heavily particle loaded explosive mixtures. Significant interest has developed in modeling the collateral effects produced by metal-loaded mixtures in which the metal load contributes significantly to the mass and volume of the explosive. These types of simulations will require new models for treating these complex mixtures. The plan is to use the discrete particulate model to represent the effects associated with the expanded material and its interaction with targets. The more condensed phases of the explosive evolution will have to be modeled using a multiple field approach to represent the metal-gas interactions. Work on the multiple field approach has begun.

Particle transport has been added to the code. This model currently allows for drag on the particles and elastic and inelastic collisions with boundaries. This feature has been extended to allow for the representation of the momentum transport between the particle and the medium. The interaction between the particle and the surrounding medium is parameterized in terms of a drag coefficient. The model has recently been updated to better represent the effects of pressure gradients as observed in strong shocks.

User Interaction

The amount of interaction with the Defense community has increased considerably. A number of analyses have been performed to serve as examples of the utility of ALE3D for certain classes of problems. Computer support and a dedicated location have been allocated at LLNL for training activities. The intention is to provide individual attention to a user or a few users at a time in demonstrating how to simulate problem of interest to them. This approach has proved useful in the past and continues to be a good model for future interactions. Several organizations have requested and received versions of ALE3D in the past year.

Planned Work

ALE3D development will continue to be driven by feedback from the defense community. This has produced a focus on the areas associated with providing new and improved material models, more sophisticated structural representations, enhancement in combined effects simulations, and continued development of the parallel version of the code. Interest in simulating safety and vulnerability of weapons systems is providing the emphasis on combined thermal-chemical-mechanical modeling capabilities. Multiple physics options, more complex physical models, and the availability of multiprocessor configurations provide the motivation for the parallelization effort.

Technology Transition

ALE3D has been made available to a number of DoD facilities and contractors this year.

Organization	Contact
Eglin/AFRL/MNAC	Douglas Nance
Picatinny Arsenal	Vladimir Gold
USA Space and missile Defense Command	John Tipton
Naval Explosive Ordnance Tech Division	Richard Gold
NSWC Dahlgren	Robert Nance
Naval Research Laboratory	Andrew Geltmacher
Foils engineering	Marshall Eck
ANALYTIX Corp.	Heros Noravian
Computer Aided Engineering Associates	Steven Hale

Relationship to Ongoing Work in DOE/Services/OSD

A 3D ALE code with some of the features of ALE3D is under development at SNL.

Benefits to DOE/DoD

A combination of economic and political factors has placed an increased emphasis on modeling and simulation in DOE and DoD design and evaluation activities. The 3D code development activity supported here is focussed on support of those activities, particularly in the areas of multi-disciplinary and full-system simulations.

Milestones

Task B: ALE3D Development