REPORT DOCUMENTATION PAGE

Form Approved
OMB NO. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE

3. REPORT TYPE AND DATES COVERED
FINAL 01 Jul 92 - 31 Dec 97

4. TITLE AND SUBTITLE
Dynamic Behavior of Ductile Materials

5. FUNDING NUMBERS
DAAL03-92-G-0108

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
ARO 30348.29-MS-UR1

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12 b. DISTRIBUTION CODE

20010222 046

13. ABSTRACT *(Maximum 200 words)*

A comprehensive and multidisciplinary research program centered on the fundamental study of the dynamic response and failure modes of a broad class of conventional and advanced ductile materials. This research program is founded on four important areas:

a) the unique and novel experimental facilities for dynamic testing established at UCSD;
b) a balanced multidisciplinary program with investigators of combined expertise and prominence in the fields of materials, mechanics and computational and experimental methods;
c) a continuing interaction with U.S. Army research laboratories (primarily, but not exclusively, BRL, MTL, and ARDEC) which serves to maintain the relevance of the program, transfer to the Army its most significant accomplishments, and provide a vehicle (forum) for the continuing training of U.S. Army scientists;
d) a vital and productive educational environment for future scientists in the field of dynamic behavior of materials.

The research program addresses materials of current interest to the Army (tungsten, tungsten composites, tantalum, advanced steels and copper), as well as novel materials and concepts (nanocrystalline metals, and metal-matrix composites. The specific programs are developed in a multi-disciplinary, multi-investigative mode, encompassing experimental, analytical, and microstructural characterization components. Through comprehensive testing and analysis, physically-based constitutive models are developed which will enable the prediction of the microstructural response and its tailoring for optimization of performance in Army systems.

14. SUBJECT TERMS
Ductile materials, High-Strain-Rates, Penetration

15. NUMBER IF PAGES
32

16. PRICE CODE

17. SECURITY CLASSIFICATION OR REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

DTIC QUALITY INSPECTED 1

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

FINAL PROGRESS REPORT

ARO Proposal Number: 30348-MS-URI
Period Covered by Report: 1992 July 1 - 1997 December 31
Title of Proposal: *Dynamic Behavior of Ductile Materials*
Contract or Grant Number: DAAL-03-92-G-0108
Authors of Report: Dr. S. Nemat-Nasser, M.A. Meyers and K.S. Vecchio

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STATEMENT OF THE PROBLEM STUDIED

The research objectives of this URI included:

1) In-depth understanding through microscopic analysis of the fundamental mechanisms of flow and failure modes of ductile materials, focusing on tantalum, tantalum-tungsten alloys, tungsten and tungsten composites, copper, and certain superalloys.
2) Creation of novel experimental techniques for controlled measurement of the response of the considered class of metals, over strain rates from 10^{-5} to greater than 10^{4}/sec. and temperatures from -200 to greater than 1,000°C, with strains exceeding a hundred percent.
3) Development of physically-based constitutive models based on both continuum mechanics and crystal plasticity, for the considered class of metals.
4) Development of computational algorithms for implementation into large-scale computer codes.
5) Model verification through simulation of controlled experiments.
6) Extensive interaction with Army laboratories and scientists, and technology transfer in both directions.
7) Education of young scientists in this area of research encourages them to join Army laboratories.

We are pleased to report that we have succeeded in achieving all these goals rather well, exceeding our own expectations in several areas. We have developed an in-depth understanding of the high strain-rate, high-temperature behavior of tantalum and tantalum-tungsten alloys, with strains exceeding 900%. Similarly, we have made good progress in understanding, modeling, and experimentally quantifying the dynamic response of copper and 230 and 180 Hayes superalloys. We have developed new Hopkinson facilities for recovery tests at various temperatures, and in this manner are now able to construct *isothermal* stress-strain curves of metals at high strain rates and elevated temperatures. We have implemented two new experimental methods to investigate the high-strain, high-strain-rate response of ductile metals: a) The hat-shaped technique, which enables controlled and prescribed true effective strains up to 9. This technique can be applied at temperatures from 77 to 1300k; and b) The thick-walled cylinder technique, which enables true effective strains of up to 4. This technique has been successfully applied to the plastic deformation of monocrystals, and polycrystals, with emphasis on shear localization and the anisotropy of plastic flow. We have developed dislocation-based constitutive models for tantalum, tantalum-tungsten alloys, and copper, which accurately simulate the high strain-rate, high-temperature response of these materials, even to extreme strain levels. We have developed a novel, dislocation-based crystal-plasticity model for tantalum and have shown it to accurately predict the observed response, with very few constitutive parameters, which are fixed at the outset. We have developed a novel constitutive algorithm, which is both accurate and remarkably efficient, for calculation of high strain, high strain-rate deformation of metals. We have had a very healthy and mutually rewarding exchange with Army laboratories, involving frequent visits and continued scientific collaboration. We have constructed, for ARL, a state-of-the-art tension *recovery* Hopkinson bar and at this writing it will soon be delivered to ARL. We have educated more than half a dozen scientists, two of whom are currently employed at ARL (Drs. Jerry LaSalvia and Scott Schoenfeld).

Chart 1 provides an overview of our research strategy.

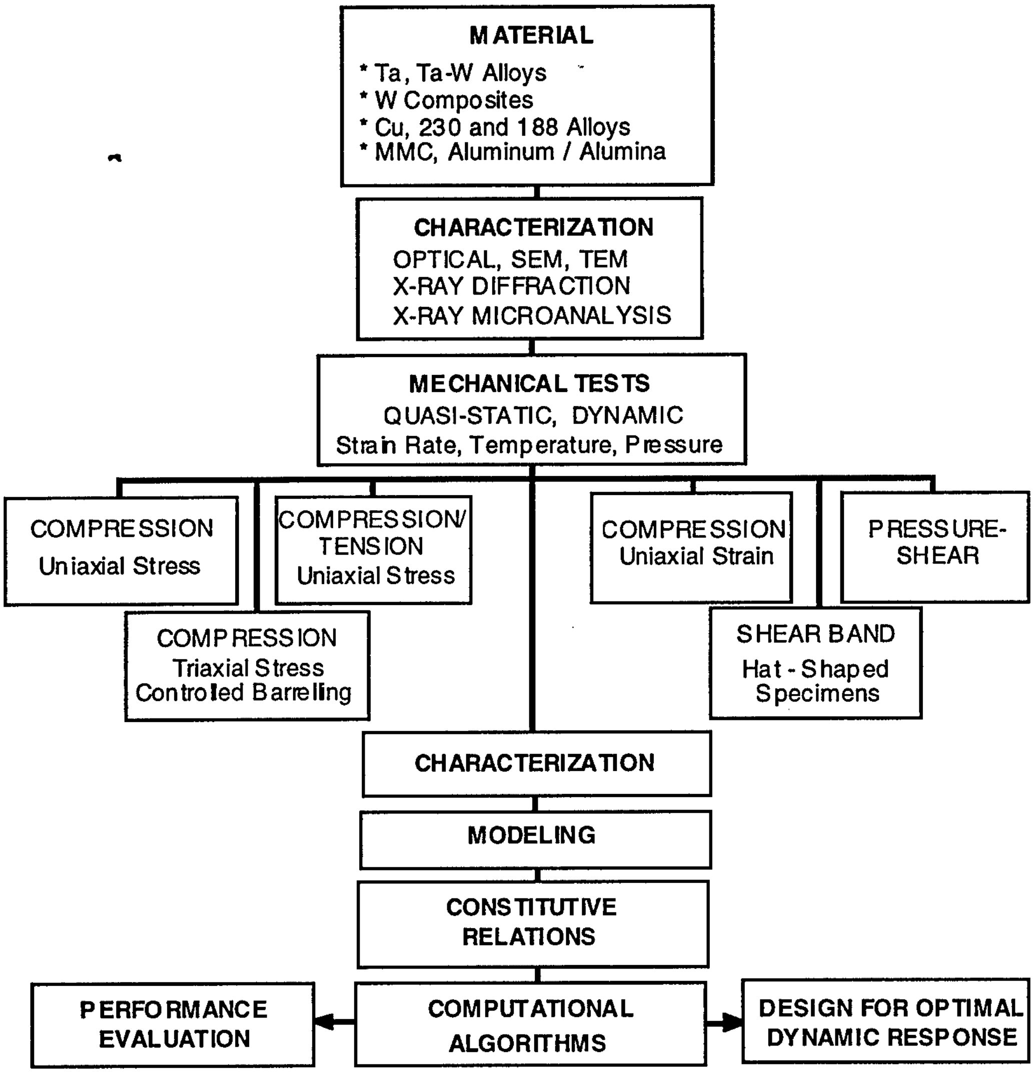

Chart 1: research strategy and materials of interest

SUMMARY OF MOST IMPORTANT RESULTS

This report provides a detailed account of the contributions of the group. Approximately sixty three publications have emerged from this effort.

1. *Experimental*

Through coordinated recovery experiments, we have sought to understand and develop capabilities to predict dynamic deformation and failure modes of a number of relevant ductile materials at high strains, high strain rates, and over a broad range of temperatures. Focus has been on tantalum, tungsten, tantalum-tungsten alloys, and tungsten composites, as well as some superalloys, copper, and aluminum/alumina composites. Both unshocked and shocked materials have been studied. Recovery experiments have been developed and performed on these materials and, through microstructural characterization, relations between microstructure, substructure evolution, and high strain-rate properties have been explored. Based on this, physically-based micromechanical, as well as phenomenological models have been developed.

1.1. Novel High Temperature Recovery Hopkinson Technique

The details of the UCSD Hopkinson recovery techniques are given in Nemat-Nasser, Isaacs, and Starrett (1991). Here, we briefly outline the enhancement of UCSD's recovery compression technique.

The Enhanced UCSD Recovery Technique

For high strain-rate tests at elevated temperatures, it is necessary to heat the sample to the required temperature, while keeping the incident and transmission bars at suitably low temperatures. If the bars are in contact with the specimen within the furnace, their temperature will increase, having a variable distribution along the bars. This may affect the bars' elastic properties and hence, the stress pulses. Moreover, the bars being good heat conductors (usually of maraging steel), the considerable heat loss that occurs makes controlling the experiment difficult. To avoid these and related difficulties, the bars are kept outside the range of the heating unit in the furnace, while keeping the specimen at the center of the furnace. The bars are then brought into contact with the specimen, microseconds before the stress pulse reaches the end of the incident bar. This is accomplished by two *moving arms, which* are activated by the same gas gun that propels the striker bar toward the incident bar. The area of its piston and the gas pressure in the breach controls the motion of the moving arms. In the UCSD design, the bars are brought into contact with the specimen a few microseconds before the elastic pulse traveling in the incident bar loads the sample.

Suitable wires attach the sample to a sleeve, which is a thin tube. The moving arms then move the transmission bar, bring it in contact with the sample, and then the sample, the sleeve, and the transmission bar are brought in contact with the incident bar.

1.2 Hat-Shaped Experiments: Dynamic Recrystallization

To test as-received and shocked materials at high strains (up to several hundred percent), and at high strain rates (up to 50,000/s and greater), we have employed hat-shaped specimens. In this test, an adiabatic shearband is generated in a controlled geometry under an imposed shear stress which may be chosen to be accompanied by compression, hence closely simulating the loading environment of interest. The surrounding cooler material, in less than one millisecond then quenches the shearband. The sample can be sectioned and its microstructure studied. Our team has been successful in using this technique to explore the fundamentals of dynamic recrystallization and other microstructural changes that may take place at high strain rates and during large straining.

Existing theories for recrystallization kinetics have been applied to the deformation conditions during shearbanding and were found to be inadequate to explain the observed grain sizes. Based on the temperature-time profile of the actual shearband, the diffusion kinetics of classical recrystallization models indicate that the observed recrystallized grain sizes within shearbands (0.1-0.2mm) are 5-7 orders of magnitude larger than those predicted from these models. As such, a new model is being developed, based on a modification of the subgrain rotation-coalescence model for recrystallization, whereby a significant portion of the normally diffusion-assisted subgrain rotation is achieved through a deformation-assisted lattice rotation. This model is being tested through calculation of lattice rotations of subgrains based on the deformation history of the shear band.

1.3 Thick-Walled Cylinder Collapse Experiments

- The self-organization of shearbands in stainless steel and titanium was established by means of experiments in which the collapse of a thick-walled cylinder enabled controlled strain gradients, strains, and strain rates. This geometry lends itself very well to analysis, and experimental results were successfully compared with shearband spacing predictions of models proposed by Grady-Kipp and Ockendon-Wright.

- *Experimental and Computational Study of Tantalum and Copper using the Cylinder Collapse Method*

High-strain, high-strain-rate deformation of most metals, is generally accompanied by strain localization and adiabatic shearbanding. To understand and model this phenomenon, thick-walled circular cylinders have been collapsed quasi-uniformly, by explosively generated energy; placing the explosive charge coaxially with the thick-walled cylinder performed this. Shear strains of up to 10, at strain rates exceeding 10^4/s are obtained in an axisymmetric plane-strain configuration. The high-strain, high-strain-rate deformation process generates thermal heating which may produce significant microstructural changes. Computational simulations have accompanied the experiments.

Grain-scale localization produced by anisotropic plastic flow and localized recovery and recrystallization is observed at the higher plastic strains *(g > 4)*. Residual tensile "hoop" stresses are generated near the central hole region upon unloading; this results in fracturing along shear localization bands.

- *Self-organization in the Initiation of Adiabatic Shear Bands*

The radial collapse of a thick-walled cylinder under high-strain-rate deformation ($\sim 10^4\ s^{-1}$) was used for the investigation of shear-band initiation and pattern development in titanium. Experiments were carried out in which the collapse was arrested at two stages, in order to observe the initiation and propagation of shear bands. The occurrence of shear bands to accommodate general plastic deformation in response to external tractions is a collective phenomenon, because their development is interconnected. The bands were observed to form on spiral trajectories and were periodically spaced. The spacing of the shear bands decreased with the progression of collapse, and was equal to approximately 0.6 mm in the final stage of collapse. The shear-band spacing was calculated from two existing models, based on a perturbation analysis and on momentum diffusion. The values of 0.52 and 3.3 mm were obtained with material parameters obtained for the same material in quasi-static and dynamic experiments for different strain rates. The predictions are found to give a reasonable first estimate for the actual spacings. The detailed characterization of the shear-band front leads to an assessment of the softening mechanisms inside a shear localization region.

The initiation of localization takes place at favorably oriented grains and becomes gradually a continuous process, leading eventually to dynamic recrystallization.

1.4 Dynamic Recrystallization

An important result of the research effort is that dynamic recrystallization is a key mechanism under high strain, high strain rate deformation of copper and tantalum. This regime is important in shaped charges and EFPS. Mechanisms for dynamic recrystallization have been identified and the process is being modeled from both a dislocation and crystal plasticity points-of-view.

- *Shear Localization and Recrystallization in High-Strain, High-Strain-Rate Deformation of Tantalum*

Tantalum was subjected to high plastic strains (engineering shear strains γ between 0 and 90) at high strain rates ($> 10^4$ s^{-1}) in an axisymmetric plane strain configuration. Tubular specimens, embedded in thick-walled cylinders made of copper, were collapsed quasi-uniformly by explosively-generated energy; placing the explosive charge co-axially with the thick-walled cylinder performed this. The high strains achieved generated temperatures, which produced significant microstructural change in the material; these strains and temperatures were computed as a function of radial distance from the cylinder axis. The microstructural features observed were: (i) dislocations and elongated dislocation cells ($\varepsilon_{eff} < 1$, $T < 600$ K); (ii) subgrains ($1 < \varepsilon_{eff} < 2$, $600\ K < T < 800\ K$); (iii) dynamically recrystallized micrograins ($2 < \varepsilon_{eff} < 2.5$, $800\ K < T < 900\ K$); and (iv) post-deformation recrystallized grains ($\varepsilon_{eff} > 2.5$, $T > 1000\ K$). Whereas the post-deformation (static) recrystallization takes place by a migrational mechanism, dynamic recrystallization is the result of the gradual rotation of subgrains coupled with dislocation annihilation. A simple analysis shows that the statically recrystallized grain sizes observed are consistent with predicted values using conventional grain-growth kinetics. The same analysis shows that the deformation time is not sufficient to generate grains of a size compatible with observation (0.1 - 0.3 μm). A mechanism describing the evolution of the microstructure leading from elongated dislocation cells, to subgrains, and to micrograins is proposed. Grain-scale localization produced by anisotropic plastic flow and localized recovery and recrystallization was observed at the higher plastic strains ($\varepsilon_{eff} > 1$). Residual tensile "hoop" stresses are generated near the central hole region upon unloading; this resulted in ductile fracturing along shear localization bands.

- *Dynamic Recrystallization in High-Strain, High-Strain-Rate Plastic Deformation of Copper*

When copper is deformed to high strain ($\gamma \sim 3 - 4$) at high strain rates ($\sim 10^4$ s^{-1}) a microstructure with grain sizes of ~ 0.1 μm can be produced. It is proposed that this microstructure develops by dynamic recrystallization, which is enabled by the adiabatic temperature rise. Shock-loading the material, and thereby increasing its flow stress can enhance the propensity for dynamic recrystallization. The grain size-flow stress relationship observed after cessation of plastic deformation is consistent with the general formulation proposed by Derby [*Acta metall. mater.* **39**, 955 (1991)]. The temperatures reached by the specimens during dynamic deformation are calculated from a constitutive equation and are found to be, for the shock-loaded material, in the 500-800 K range; these temperatures are consistent with static annealing experiments on shock-loaded specimens, that show the onset of static recrystallization at 523 K. A possible recrystallization mechanism is described and its effect on the mechanical response of copper is discussed.

1.5 Influence of Stacking Fault Energy on Shock Hardening Propensity and Strain Localization in Cu-Al Alloys

This project is still being pursued with graduate student Aashish Rohatgi under the guidance of Prof. K. Vecchio. The research is aimed at understanding to influence of a materials stacking fault energy on its propensity to shock harden and strain localize. These two characteristics are related to the evolution of substructure in these materials. Two different shock pressures are being investigated: a low pressure of 10 GPa, and a higher pressure of approx. 40 GPa. The low pressure experiment has been completed through collaboration with Rusty Gray at Los Alamos and specimens are being characterized. The high pressure was tested recently at New Mexico Tech.; results from both these shock experiments are forthcoming. Five Cu-Al alloys are being investigated ranging from pure copper to Cu-6Al. The constitutive response of the as-received materials and the low pressure shocked samples has been documented, and reload tests of the high pressure shocked samples is underway. The characterization of the dislocation configurations within the various samples is being conducted using a novel ultrasonic technique involving analysis of high frequency wave attenuations. This technique will enable more detailed and quantitative measurements of the dislocation variations among the different alloys. It is expected that the student will complete his research by the end of 1997.

1.6 Influence of Peak Pressure and Temperature on the Structure / Property Response of Shock-Loaded Ta and Ta-10W

The deformation behavior and substructure evolution of unalloyed-Ta and Ta-10W under quasi-static conditions has been compared to their respective response when shock pre-strained to 20 GPa at 25°C as well as to unalloyed-Ta shocked to 7 GPa at 25°C, 200°C and 400°C. The reload yield behavior of shock-prestrained Ta and Ta-10W did not exhibit enhanced shock hardening when compared to their respective quasi-static stress-strain response at an equivalent strain level. In addition, the reload yield behavior of Ta shock prestrained to 7 GPa at 200 or 400°C was found to exhibit increased hardening compared to the shock prestraining at 25°C. The quasi-static substructure evolution and shock-hardening responses of Ta and Ta-10W were investigated via TEM. The dislocation substructures in both materials and at each strain rate condition and temperature were similar and consisted primarily of long, straight, (a/2)<111> type screw dislocations. The propensity for long, straight screw dislocations, irrespective of the loading condition supports the theory of strong Peierls stress control on defect generation and defect storage. The substructure evolution and mechanical behavior of Ta and Ta-10W is discussed in terms of defect storage mechanisms and compared to the mechanisms operative in FCC metals.

1.7 Shock-loading Response of 6061-T6 Aluminum Metal-Matrix Composites

The purpose of this research was to systematically study the influence of peak-shock pressure and second-phase reinforcement on the structure/property response of shock-loaded 6061-T6 Al-alumina composites. The reload stress-strain response of monolithic 6061-T6 Al, used as a baseline for comparison, showed no increased shock hardening compared to the unshocked material deformed to an equivalent strain. The reload stress-strain response of the shock-loaded 6061-T6 Al-

alumina composites exhibits a lower reload yield strength than the flow stress of the starting composites. The degree of strength loss was found to increase with increasing shock pressure. Wavespeed measurements of shock-prestrained specimens showed no degradation compared to unshocked specimens indicating that particle cracking had not occurred under shock. This result was supported by optical metallography which did not reveal cracked particles or particle decohesion in the shock-prestrained samples. The reload stress-strain response of the shock-prestrained composites, after re-solutionizing and T6 reaging, showed that the composites recovered their full as-received preshock stress-strain responses. This result supports that the observed degradation in reload strength was attributable to matrix microstructural changes resulting from the shock. TEM examination of the shock-loaded microstructures revealed that the matrix regions adjacent to the particle/matrix interface had undergone significant recovery and partial recrystallization resulting from the shock. This type of near-interface substructure is in stark contrast to the heavily-dislocated near-interface dislocation substructure of the as-received composites. The loss of dislocation density (i.e. strain hardening) in the near interface matrix region, resulting from the shock, highlights the importance of the thermally-introduced dislocation substructure changes in establishing the strength of metal-matrix composites.

1.8 Dynamic Bauschinger Effect

An experimental investigation of the “Bauschinger effect” in materials under dynamic loading conditions is presented. In this study, a tension split Hopkinson bar with a momentum trap is used to subject a tensile specimen to a single high-strain-rate tension pulse of known magnitude and duration. The uniformly deformed gauge length of the tension specimen is then sectioned and loaded in a compression split Hopkinson bar with a momentum trap, at essentially the same strain rate as that of the initial tension test. Comparison was made between these high strain-rate Bauschinger experiments and similar tests carried out under quasi-static conditions. Two different material microstructures were examined: solid-solution strengthened alloys and precipitation-strengthened alloys. The Bauschinger effect is found to be a function of the initial material microstructure, as well as strain rate.

1.9 Bauschinger Effect in Haynes 230 Alloy: Influence of Strain Rate and Temperature

Quasi-static and dynamic Bauschinger behavior in HAYNES 230 Alloy is examined. At low strain rate (10^{-3}/s), the as-received 230 alloy does not show a drop in flow stress upon stress reversal, i.e. no Bauschinger effect is displayed. At high strain rate (10^{+3}/s), a drop in flow stress of 160 MPa was observed upon stress reversal. In contrast, the precipitation-strengthened condition of 230 alloy exhibited a Bauschinger effect in both low and high-strain-rate stress-reversal experiments. The magnitude of the Bauschinger effect was found to increase with increasing strain rate, forward strain and decreasing temperature. The substructure evolution accompanying the forward loading cycles was investigated by transmission electron microscopy and is related to the back stresses developed. The increased Bauschinger stress drop observed at high strain rate and/or low temperature was correlated to an increased degree of planar slip under these deformation conditions.

1.10 Role of Interstitials in Powder Metallurgy Processed Tantalum Alloys

This project is examining the role of interstitials, primarily oxygen; hydrogen and nitrogen, on the structure-properties of Ta materials produced by powder metallurgy. Los Alamos National Lab and Cabot Corp. are providing the materials, with additional funding being provided by Los Alamos. Several Ta alloys are being investigated with a range of oxygen, nitrogen, and hydrogen levels with the intent of determining the individual and combined effects of these interstitials on the strength of Ta. The work is being carried out by Dr. Strutt and Prof. Vecchio at UCSD and Sherri R. Bingert and George T. Gray, III at Los Alamos National Lab.

1.11 Compositional Banding in Ta-10W Alloys

This work is a small project as part of the larger Ta alloys work being pursued by Prof. Vecchio. Narrow striations parallel to the rolling plane of plate Ta-10W material have been observed under optical microscopy of as-polished sections. These striations have been correlated to compositional variations of ±0.5 wt.% W through very thorough microprobe analysis. The striations are being correlated with composition segregation present in the original dendrite cast structure. A section of a Ta-10W cast ingot has been obtained from Cabot Corp. and was characterized to determine the degree of segregation in the original casting. Sections of the cast plate have been subsequently upset forged to document the evolution of the segregation into the striations present in the rolled plates.

1.12 High Strain, High-Strain-Rate Behavior of Tantalum

Tantalum plate produced by a forging-rolling sequence was subjected to high plastic shear strains ($\gamma = 1 \rightarrow 5.5$) at high strain rates ($\sim 4\times10^4$ s^{-1}) in two experimental configurations: (a) a special hat-shaped geometry and (b) thin disks deformed in a split Hopkinson bar. In parallel experiments, the constitutive behavior of the same material was established through quasi-static and dynamic compression tests at ambient and elevated temperatures. The microstructure generated at high strain rates and retained by rapid cooling from a narrow (200 μm) deformation band progresses from dislocated, to elongated cells, to banded structures, and finally, to subgrains as the shear strain increases from zero to 5.5. The temperature rise predictions from the constitutive description of the material indicate that the temperature reaches values of 800 K, and it is proposed that thermal energy is sufficient to produce a significant reorganization of the deformation substructure, leading to a recovered structure.

1.13 High-Strain-Rate Response of Tantalum at Low Temperatures

Tantalum was subjected to high-strain-rate (1000 ~ 7000 / sec) deformation at low temperatures (77 and 190 K). The interrupted testing method was applied to obtain the iso-thermal deformation response at high strain rates. Mechanical twinning was observed at both temperatures, in accordance with predictions that twinning occurs when a threshold stress is reached. Shear localization was observed in the specimens with the plastic strain 0.2 at 77 K and 0.57 at 190 K. The parameters of Zerilli - Armstrong equation were established with the data at room temperature and the quasi-static data at low temperatures.

1.14 Effect of Strain Rate on Plastic Flow and Failure in Polycrystalline Tungsten

The objective of this investigation was to establish the effect of strain rate on the mechanisms of flow and failure of polycrystalline tungsten under compressive loading. Polycrystalline tungsten (less than 100 ppm impurities) was subjected to different heat treatments to yield different grain morphologies and tested at quasi-static ($3\cdot10^{-3}s^{-1}$) and dynamic (10^3 to $4\cdot10^3$ s^{-1}) strain rates. Three mechanisms of deformation were identified and evaluated: slip, twinning, and intergranular cracking. Whereas plastic flow by slip has considerable strain-rate sensitivity in tungsten (typical for BCC metals), the cohesive strength of the grain boundaries was found to decrease with heat treatment temperature, but was insensitive to strain-rate changes. Low-strain-rate deformation yielded limited damage at strains as high as ~0.25, whereas high strain-rate deformation led to catastrophic failure at strains between 0.05 to 0.10. Slip and grain-boundary decohesion are competing deformation mechanisms, the former being favored under quasi-static and the latter under high-strain rate conditions. As a consequence, the material undergoes a ductile-to-brittle transition as the strain rate is increased from 10^{-3} to 10^3s^{-1}. Optical and scanning electron microscopy as well as quantitative statistical analysis of micro, meso and macrocracks confirm a wing-crack mechanism formation, which is analyzed in terms of the Ashby-Hallam [*Acta Metall.* **34**, 511 (1986)] treatment, and damage initiation due to grain-boundary voids, which is analyzed by means of the Sammis-Ashby [*Acta Metall.* **34**, 497 (1986)] treatment. The results and analysis confirm that damage evolution is a strong function of grain-boundary cohesive strength. The interactions between microcracks and twins are characterized, and there is both evidence of fracture initiation at twins (intergranular cracks), and twin initiation at cracks (transgranular cracks). Twinning of the material at high strain rates does not play a significant role in damage evolution.

1.15 The Effect of Grain Size on the High-Strain, High-Strain-Rate Behavior of Copper

Copper with four widely differing grain sizes was subjected to high-strain-rate plastic deformation in a special experimental arrangement in which high shear strains of approximately 2 to 7 were generated. The adiabatic plastic deformation produced temperature rises in excess of 300 K, creating conditions favorable for dynamic recrystallization, with an attendant change in the mechanical response. Preshocking of the specimens to an amplitude of 50 GPa generated a high dislocation density; twinning was highly dependent on grain size, being profuse for the 117- and 315- μm grain size specimens and virtually absent for the 9.5-μm grain size specimens. This has a profound effect on the subsequent mechanical response of the specimens, with the smaller grain-size material undergoing considerably more hardening than the large grain-size material. A rationale is proposed which leads to a prediction of the shock threshold stress for twinning as a function of grain size. The strain required for localization of plastic deformation was dependent on the combined grain size/shock-induced microstructure, with the large grain-size specimens localizing more readily. The experimental results obtained are rationalized in terms of dynamic recrystallization, and a constitutive equation is applied to the experimental results; it correctly predicts the earlier onset of localization for the large grain-size specimens. It is suggested that the grain-size dependence of shock response can significantly affect the performance of shaped charges

2. *Analytical and Computational Modeling*

- The analytical modeling included collaborative work with Dr. T. Wright, on two general research areas: (1) an analysis of the collective behavior of shearbands where the effort has been directed at predicting the collective configuration of the shearbands developed in the thick-walled cylinder-collapse experiments; and (2) an effort to develop a matched asymptotic analytic solution for a shearband growing into a viscoplastic solid.
- The computational effort has focused on two areas: (1) computational modeling of high strain-rate deformation of single- and polycrystalline solids (e.g., tantalum and copper), using crystal plasticity; and (2) implementation of the new algorithm developed by Nemat-Nasser and coworkers at UCSD, into DYNA3D and DYNA2D and their use to simulate the hat-shaped and other high strain-rate experiments. We have made considerable progress in both areas. In particular, the effort to implement the new algorithm into DYNA3D has been successfully completed.

2.1 Crystal Plasticity Modeling of Polycrystalline Tantalum

A model is developed for dynamic deformation of polycrystalline tantalum based on crystal plasticity with due account of the short- and long-range barriers which the dislocations must overcome in their motion that leads to plastic slip of various slip systems. For each single crystal, forty-eight potentially active slip systems are included, with {110}-, {112}-, and {123}-families of slip planes and the <111>-family of slip directions. A new efficient and accurate algorithm is developed for the single-crystal calculations. Using a Taylor averaging method, the polycrystal response is calculated and the results are applied to predict the response of commercially pure Ta, over a broad range of strain rates (10^{-3} to 4 $\times 10^{4}$/s) and temperatures (77 to 1300K), with strains exceeding 100%.

The results are compared with extensive experimental data, which have been produced using UCSD's recovery Hopkinson technique.

2.2 Crystal Plasticity Modeling of Single Crystal Copper

An algorithm is proposed for the calculation of the finite deformation of fcc single crystals, using a rate-dependent slip model. The method also applies bcc and hcp crystals. The history of the deformation is divided into three regimes, depending on the number of *active* slip systems and a computational strategy is proposed for each regime. The proposed algorithm uses a combination of the forward-gradient and the plastic-predictor elastic-corrector methods. The efficiency and the accuracy of the proposed algorithm are demonstrated by comparing the results with those of the conventional method.

2.3 Crystal Plasticity Modeling of Copper

Localization of the inelastic flow and crack initiation in fcc single crystals are studied experimentally and by numerical simulations, focusing on the anisotropic inelastic response of the crystal, and the mechanisms of possible crack initiation and growth, produced upon unloading by the residual inhomogeneous plastic strains. Hollow circular cylinders of single-copper are subjected to externally applied explosive loads which cause the collapse of the cylinder; this procedure is called the thick-walled cylinder (TWC) method. Then, numerical simulations are performed to understand the deformation process which leads to localized deformation, and tensile cracking when partial collapse is followed by unloading. Various loads and initial orientations of the lattice are examined in these numerical simulations in order to study their effects on the flow localization and crack initiation phenomena.

2.4 Kinetics Modeling of Microstructural Evolution during Shear Banding

This research was primarily a material modeling project focused at developing an understanding of the mechanism responsible for the formation of recrystallized grains observed in shear bands formed under high strain, high strain-rate conditions. This work was being carried out by Joy Hines who was supported primarily through a fellowship from the university. Existing theories for recrystallization kinetics have been applied to the deformation conditions during shear banding and were found to be inadequate to explain the observed grains sizes. Based on the temperature-time profile of the actual shear band, the diffusion kinetics of these models indicates that grain sizes 10^5 to 10^7 times smaller would occur. As such, a new model was developed based on a modification of the subgrain rotation-coalescence model for recrystallization, whereby a significant portion of the normally diffusion-assisted subgrain rotation is achieved through a deformation-assisted lattice rotation. This model was tested through calculation of lattice rotations of subgrains based on the deformation history of the shear band. These calculations have indicated that this subgrain rotation mechanism can yield misorientations between subgrains significantly greater than 25 degrees. The boundaries of this highly misoriented subgrain can then undergo dislocation recovery depending on diffusion kinetics of the particular shear band materials. The observation of recrystallized grains within the shear bands of various materials is consistent with the subgrain boundary dislocation recovery kinetics following shear band formation.

2.5 Modeling the Mechanical Behavior of Tantalum

A crystal plasticity model was developed to simulate the large plastic deformation and texture evolution in tantalum over a wide range of strain-rate. In the model, a modification of the viscoplastic power-law for slip and a Taylor interaction law for polycrystals is employed which account for the effects of strain hardening, strain-rate hardening and thermal softening. A series of uniaxial compression tests in tantalum at strain-rates ranging from $10^{-3}s^{-1}$ to 10^4s^{-1} were conducted and used to verify the model's simulated stress-strain response. Initial and evolved deformation textures were also measured for comparison with predicted textures from the model. Applications of this crystal plasticity model are made to examine the effect of different initial crystallographic textures in tantalum subjected to uniaxial compression deformation or biaxial tensile deformation. Further modification of this model included a description for the thermal-elastic-viscoplastic behavior of Ta single crystals along with an associated polycrystal averaging scheme. The description incorporates a temperature dependent model for pencil glide on the planes of maximum resolved shear stress. Calculated stress-strain data and texture evolution for this modified model were compared to those of the earlier restricted glide model and to experimental data. The new model yielded similar results in terms of texture and flow curve predictions, yet is significantly more efficient computationally that the previous model. This work was carried out in collaboration with Said Ahzi, B. J. Lee, and Scott Schoenfeld.

2.6 Shock-Induced Deformation Twinning in Tantalum

Shock-wave deformation of tantalum to a pressure of 45 GPa and duration of 1.8 μs generates profuse twinning. The post-shock mechanical response is significantly affected, with shock hardening exceeding the expected hardening due to the transient shock strain $\varepsilon_S = \frac{4}{3}\ln\frac{V}{V_0}$; this enhanced hardening, and other alterations in response, are attributed to the barriers presented to plastic deformation by the deformation twins.

A constitutive model is proposed that predicts the threshold shock stress for mechanical twinning; it is based on the application of the Swegle - Grady relationship between shock stress and strain rate to constitutive equations describing the critical stress for slip and twinning. This constitutive model incorporates grain-size effects and predicts a threshold twinning stress that is a function of temperature and grain size; predictions of the model are in qualitative agreement with experimental results.

2.7 Constitutive Description of Work- and Shock-Hardened Copper

Constitutive models are an essential part of large-scale computational codes which describe material behavior, since they provide the relationship between stress, strain, strain rate, and temperature. However, plastic deformation is an irreversible and path-dependent process, and a number of parameters affect the development of the deformation structure and as a consequence, the mechanical response. The stress state, strain rate, and temperature affect the evolution of the microstructure, and the strain, current temperature and strain rate alone are frequently not sufficient to describe it.

Experimental results on cold-worked and shock-hardened copper reveal the occurrence of dynamic recrystallization at temperatures of ~700 and 600 K, respectively. The available empirical constitutive equations do not generally account for such microstructural changes, and this leads to a poor fit between the experimental results and the predictions. A modified constitutive equation incorporating a reducer function to represent dynamic recrystallization was applied to work hardened and shock-hardened copper, providing a much improved fit.

3. Microstructural Analysis

Extensive microscopy has been an integral part of our research to relate the microstructure to the mechanical properties and to identify the essential micromechanisms responsible for the overall behavior of the material. This included optical microscopy, SEM, TEM, and X-ray diffraction.

Our focus has been a careful understanding of the dislocation and twinning substructure, their evolution during high strain-rate deformation and its effect on the properties. In the case of preshocked materials, the shock-induced microstructure is examined for its effect on the subsequent response.

3.1 Microstructure of High-Strain-Rate Deformed Tantalum

Hat-shaped specimens of polycrystalline tantalum are subjected to high plastic shear strains ($\gamma = 170$ to 910%) at strain rates exceeding 5×10^4/s in a compression split Hopkinson bar. The dynamic shear tests are performed at room and 600K initial temperatures, under adiabatic and quasi-isothermal conditions, using UCSD's recovery Hopkinson technique. The microstructure of the post-test specimens is examined with transmission electron microscopy (TEM). The plastic deformation is highly concentrated, producing a narrow shear-localization region of approximately 200μm in width. Slip of perfect screw dislocations, on the {110} primary planes along the <111> directions, is found to be the dominant deformation mechanism. Dynamic recovery takes place in the shear-localization regions of all adiabatically tested specimens, and evidence of dynamic recrystallization is observed in the specimen deformed to a shear strain of 910% at a 600K initial temperature. The substructures of the adiabatically tested specimens include well-defined dislocation arrays, grouped dislocations, elongated dislocation cells, subgrains, and recrystallized micro-sized grains. The microstructure of isothermally tested specimens, on the other hand, features high dislocation density and inhomogeneous dislocation distribution. In light of the TEM observations, the relationship between the microstructure and shear stress, the caused of strain inhomogeneity, the estimated adiabatic temperature within the shear-localization zone, the rapid quenching of the shearband at the end of the dynamic testing, the slip characteristics of dislocations in tantalum, and the formation mechanisms of dislocation loops, are discussed.

4. Materials Development Research

4.1 Development of a New Tungsten Heavy Alloy Based on a HAYNES 230 Alloy Matrix

This project has been a major focus during the past 12 months by Prof. Vecchio. The research is directed at developing a new tungsten-based heavy alloy, which uses a Ni-Cr-W alloy as the binder phase. Prof. Vecchio has spent several weeks at Los Alamos during the past 12 months working with Sheri Bingert, Haskell Sheinberg and Paul Dunn of the Solidification Technology group to develop several different processing routes for fabrication of a large scale sample. Several cold-isostatically pressed and liquid-phase sintered samples were produced during the previous 6 month period, and were characterized in terms of their consolidation density, microstructure, and deformation behavior. Our first attempts yielded promising results with over 96% density achieved. However, significant reaction occurred between the W particles and the Ni-Cr-W alloy binder phase resulting in the binder phase containing a significant fraction of Ni_4W precipitates. These precipitates are undesirable and the processing technique was modified to provide for faster cooling to minimize this reaction. Based on the analysis of these samples, a single large body was produced containing 90% W-10% Ni-Cr-W alloy binder phase, but processed to include a quench cycle following the liquid phase sintering operation. This sample has greater than 99% density and contains no second phase precipitates within the binder phase, as verified by transmission electron microscopy. The constitutive response and shear banding propensity of this material was then investigated. Low velocity (500 m/s) penetration experiments were conducted using this new penetrator material, fired into cold-rolled steel plates. For purposes of comparison, pure W and several different WHAs (several of which were swaged or extruded rods) were fired under similar conditions to evaluate the penetration mechanics of each material. Although the depth of penetration did not vary significantly among the various materials, only the new material exhibited the desired chisel nose shear failures, which was the initial goal of this alloy development project. Additional specimens are currently being processed using the same alloy composition and processing schedule. These samples will be swaged or extruded to improve the mechanical properties of the material, and further penetration experiments are then planned. Depending on the results of this investigation, plans will be made to produce a larger specimen suitable to conduct a small-scale weapons test.

Abstracts of Un-Published Completed Papers

- "DYNAMIC CRACK GROWTH IN INELASTIC SOLIDS WITH APPLICATION TO ADIABATIC SHEARBANDS" S. Nemat-Nasser

Introduction

Asymptotic solutions of the stress and strain fields near the tip of a steadily advancing crack in an elastic-plastic solid, have been worked out by Slepyan (1976) for Mode II, and by Gao and Nemat-Nasser (1983a,b, 1984) for all three fracture modes, as well as for elastic, power-law hardening (elastic-plastic) material models; see also Nemat-Nasser and Obata (1990). Adiabatic shearbands in similar model materials have been examined analytically, mostly as one-dimensional problems; see, for example, Clifton *et al.* (1984), Wright and Batra (1985), Wright and Walter (1987), Burns (1990), Walter (1992), and Olmstead *et al.* (1994). There are many features in common between a dynamically growing crack and an advancing adiabatic shearband in an elastic-plastic solid. Here, some of these are briefly examined, focusing on near-field asymptotic solutions of these problems. Of particular interest is the effect of the assumed constitutive model on the structure of the asymptotic solutions, especially the nature of the temperature field.

- "DIRECT MEASUREMENT OF ISOTERMAL FLOW-STRESS OF METALS AT ELEVATED TEMPERATURES AND HIGH STRAIN RATES WITH APPLICATION TO TA AND TA-W ALLOYS" S. Nemat-Nasser and J. Isaacs

Abstract

A technique is developed for measuring the flow stress of metals over a broad range of strains, strain rates, and temperatures, in uniaxial compression. It utilizes a recent, enhanced version of the classical (Kolsky) compression split Hopkinson bar (Nemat-Nasser *et al.*, 1991), in which a sample is subjected to a single stress pulse of a predefined profile, and then recovered without being subjected to any other additional loading. For the present application, the UCSD's split Hopkinson bar is further enhanced by the addition of a new mechanism by means of which the incident and transmission bars of the split Hopkinson construction are moved into a constant-temperature furnace containing the sample, and gently brought into contact with the sample, as the elastic stress pulse reaches and loads the sample. The sample's temperature is measured by thermocouples which also hold the sample in the furnace. Since straining at high strain rates increases the sample's temperature, the sample is allowed to attain the furnace temperature after each controlled incremental loading, and then is reloaded, using the same stress pulse and strain rate. The technique also allows for checking any recoveries that may occur during unloading and reloading. Using several samples of the same material and testing them at the same strain rate and temperature, but different incremental strains, an accurate estimate of the material's isothermal flow stress can be obtained. Additionally, the modified Hopkinson technique allows the direct measurement of the change in the (high strain-rate) flow stress with a change of the strain rate, while the strain and temperature are kept constant, i.e., the strain rate can be increased or decreased *during* the high strain-rate test. The technique is applied to obtain both quasi-isothermal and adiabatic flow stresses of tantalum (Ta) and a tantalum-tungsten (Ta-W) alloy at elevated temperatures. These experimental results show the flow stress of these materials to be controlled by a simple long-range plastic-strain-dependent barrier, and a short-range thermally activated Peierls mechanism. For tantalum, a model which fits the experimental data over strains from a few to over 100%, strain rates from quasi-static to 40,000s^{-1}, and temperatures from -200 to 1000°C, is presented and discussed.

- "EFFECT OF SHOCK PRESTRAIN ON THE MECHANICAL BEHAVIOR OF TANTALUM AND TANTALUM-TUNGSTEN ALLOYS" D.H. Lassila, M.M. LeBlanc, and M A Meyers

Abstract

The effects of shock prestrain on the mechanical behavior and microstructure of annealed tantalum and Ta-W alloys have been examined. The test material was shocked to 45 GPa for 1.8 μs and soft-recovered such that deformation that occurred during this procedure was predominantly due to the shock loading. Mechanical characterization of the annealed and shock-recovered tantalum was performed over a wide range of strain rates (10^{-3} to 7,000 s^{-1}) in compression. Shock prestraining caused an increase in the yield and flow stress in all of the test materials. The test results suggest that the athermal component of the flow stress is altered and to some extent work hardening is exhausted. The effects of shock prestrain on the microstructure and substructure of the test material were examined using optical microscopy, which revealed features, which may be deformation twins. The results of these examinations and how they correlate with the effects of shock prestrain on mechanical behavior are discussed.

- "HIGH-STRAIN, HIGH-STRAIN-RATE RESPONSE OF ANNEALED AND SHOCKED TANTALUM" J.C. LaSalvia, Y.J. Chen, M.A. Meyers, V.F, Nesterenko, M.P. Bondar, and Y.L. Lukyanov

Abstract

Tantalum specimens of tubular geometry were subjected to large plastic shear strains (up to 1000%) at strain rates greater than 10^5 s^{-1} during their quasi-uniform collapse (partial) by explosively generated energy (i.e. thick-walled cylinder method). Experiments were performed on annealed and pre-shocked (45 GPa peak pressure and 1.8 μs pulse duration) tantalum. Optical microscopy revealed distinct features on specimen cross-sections: (1) profuse ductile cracks initiated at the inner surface surrounded by regions of highly deformed grains; (2) regions ahead of the crack-tips which do not exhibit the elongated grain morphology; (3) large statically recrystallized grains at the inner surface; (4) diffuse shear bands running from the inner to outer surfaces; and (5) regions of highly deformed grains intermixed with slightly deformed grains. The diffuse appearance of the shear bands is believed due to the strong orientation dependence of the yield stress and subsequent anisotropy of the work-hardening behavior of the individual grains. The lower bound estimated temperature near the inner surface (macroscopic shear strain $\gamma > 10$), calculated using a modified Johnson-Cook constitutive equation, exceeds the recrystallization temperature as reported in the literature. Transmission electron microscopy revealed the following substructural features: (1) elongated dislocation cells ($\gamma < 2$, $T < 600$ K); (2) dislocation subgrains ($\gamma < 6$, $T < 800$ K); and (3) dynamically recrystallized micrograins ($\gamma < 8$, $T < 900$ K). The kinetics of static and dynamic recrystallization is correlated with the observed residual grain sizes. It is concluded that the observed dynamic recrystallization probably occurs by a rotational mechanism.

- "PLASTICITY: INELASTIC FLOW OF HETEROGENEOUS SOLIDS AT FINITE STRAINS AND ROTATIONS" Sia Nemat-Nasser

Abstract

The theoretical basis of rate- and temperature-dependent finite-deformation plasticity is examined at the dislocation scale, leading to specific constitutive models for both bcc and fcc crystals. Using the results obtained through some novel experimental techniques, and for illustration, constitutive parameters are obtained for some commercially pure tantalum. Then constitutive relations are developed for single crystals (mesoscale), based on exact kinematics of crystallographic slip due to the dislocation motion, accompanied by elastic lattice distortion. The transition from the single (mesoscale) to the polycrystal (macroscale) response requires homogenization and averaging procedures. Hence, some fundamental averaging theorems applicable to finite strains and rotations, including the generalization of Eshelby's and the double-inclusion results to finite deformations, are outlined. The emphasis of the paper is to illustrate the essential roles that the heterogeneities at various scales, from nano to macro, play in defining the properties of metals.

- "INVESTIGATION OF HIGH-STRAIN, HIGH-STRAIN-RATE BEHAVIOR OF TANTALUM USING THECOLLAPSE OF A THICK-WALLED CYLINDER" V.F. Nesterenko, M.A. Meyers, J.C. LaSalvia, M.P. Bondar, Y.J. Chen, and Y.L. Lukyanov

Abstract

Tantalum was subjected to high plastic strains (shear strain γ: $0 \rightarrow 10$) at high strain rates ($\varepsilon \sim 10^4 s^{-1}$) in an axisymmetric plane strain configuration. Tubular specimens, embedded in thick-walled cylinders made of copper, were collapsed quasi-uniformly by explosively-generated energy; this was performed by placing the explosive charge co-axially with the thick-walled cylinder. The high strains achieved generated, temperature rises which produced significant microstructural changes in the material; these strains and temperatures were computed as a function of distance from the cylinder axis. The microstructures observed were; (i) dislocations and elongated cells ($\gamma < 2$, $T < 600$ K); *(ii)* subgrains ($2 < \gamma < 6$, $600 K < T < 800 K$); *(iii)* dynamically recrystallized micrograins ($6 < \gamma < 8$, $800 K < T < 900 K$); and (iv) post-deformation recrystallized grains ($\gamma > 10$, $T > 1000 K$). Grain-scale localization produced by anisotropic plastic flow and localized recovery and recrystallization was observed at the higher plastic strains ($\gamma > 4$). Residual tensile "hoop" stresses are generated near the central hole region upon unloading; this resulted in ductile fracturing along shear localized bands.

- "TENSILE FRACTURING IN DYNAMIC COMPRESSION" Sia Nemat-Nasser

Abstract

Both brittle and ductile materials can fracture under overall compressive loads. For brittle materials, microcracks are seen to develop at pre-existing microflaws and grow in the direction of maximum compression. In dynamic loadings, this phenomenon is highly strain rate dependent. The micromechanical model of Nemat-Nasser and Deng (1994), which seems to capture the essential feature of this process is briefly reviewed. Similarly, very ductile materials, such as copper and mild steel, can undergo brittle-type fracturing when subjected to high strain-rate dynamic compression which produces suitable heterogeneous plastic deformation fields, for example, by collapsing preexisting voids. Nemat-Nasser and Hori (1987) presented a model which suggests the possibility of such tension cracking. Nemat-Nasser and Chang (1990) showed in a series of experiments on single and polycrystalline copper and in mild steel, that fracturing of this kind does actually occur. These and related issues are briefly examined in this paper.

- "SELF-ORGANIZATION IN THE INITIATION OF ADIABATIC SHEAR BANDS"
  V. Nesterenko, M.A. Meyers and T. Wright

Abstract

The radial collapse of a thick-walled cylinder under high-strain-rate deformation ($\sim 10^4 s^{-1}$) was used for the investigation of shear-band initiation and pattern development in titanium. Experiments were carried out in which the collapse was arrested at two stages, in order to observe the initiation and propagation of shear bands. The occurrence of shear bands to accommodate plastic deformation in response to external tractions is a collective phenomenon, because their development is interconnected. The bands were observed to form on spiral trajectories and were periodically spaced. The spacing of the shear bands decreased with the progression of collapse, and was equal to approximately 0.6 mm in the final stage of collapse. The shear-band spacing was calculated from two existing models, based on perturbation analysis and momentum diffusion. Values of 0.52 and 3.3 mm were obtained with material parameters from quasi-static and dynamic experiments. The predictions are found to give a reasonable first estimate for the actual spacings. The detailed characterization of the shear-band front leads to an assessment of the softening mechanisms inside a shear localization region. The initiation of localization takes place at favorably oriented grains and becomes gradually a continuous process, leading eventually to dynamic recrystallization.

- "EFFECT OF STAIN RATE ON PLASTIC FLOW AND FAILURE IN POLYCRYSTALLINE TUNGSTEN"
  T. Dummer, J.C. LaSalvia, G. Ravichandran, and M.A. Meyers

Abstract

The effect of strain rate on the mechanisms of flow and failure of polycrystalline tungsten under compressive loading was established. Polycrystalline tungsten (less than 100 ppm impurities) were subjected to different grain morphologies and tested at quasi-static ($3x10^{-3}s^{-1}$) and dynamic (10^3 to $4x10^3s^{-1}$) strain rates. Three mechanisms of deformation were identified and evaluated: slip, twinning, and intergranular cracking. Whereas plastic flow by slip has considerable strain-rate sensitivity in tungsten (typical for BCC metals), the cohesive strength of the grain boundaries was found to decrease with heat treatment temperature, but was insensitive to strain-rate changes. Los-strain-rate deformation yielded limited damage at strains as high as -0.25, whereas high-strain-rate deformation led to catastrophic failure at strains between -0.05 to -0.10. It was established that slop and grain boundary decohesion are competing deformation mechanisms, the former being favored under quasi-static and the latter under high-strain-rate conditions. As a consequence, the material undergoes a ductile-to-brittle transition as the strain rate is increased from 10-3 to 103s-1. Optical and scanning electron microscopy as well as quantitative statistical analysis of micro, meso and macrocracks confirm a wing-crack mechanism formation, which is analyzed in terms of the Ashby-Hallam [*Acta Metall.* **34**, 511 (1986)] treatment, and damage initiation due to grain-boundary voids, which is analyzed by means of the Sammis-Ashby [*Acta Metall.*34. 497, (1986)] treatment. The results and analysis confirm that damage evolution is a strong function of grain-boundary cohesive strength. The interactions between microcracks and twins are characterized, and there is both evidence of fracture initiation at twins (intergranular cracks), and twin initiation at cracks (transgranular cracks). Twinning of the material at high strain rates does not play a significant role in damage evolution.

- "A MODEL FOR RECRYSTALLIZATION IN ADIABATIC SHEAR BANDS" J.A. Hines, K.S. Vecchio and S. Ahzi

Abstract

A mechanical subgrain rotation is proposed to account for the recrystallized grains which have been observed to form in adiabatic shear bands in a number of materials. The model is based on a 'bicrystal' approach using crystal plasticity theory to predict the evolution of subgrain misorientations. These mechanically-induced rotations are shown to occur at the high strain rate associated with adiabatic shear band formation. Recrystallized grain formation is proposed to occur by the formation and mechanical rotation of subgrains during deformation, coupled with boundary refinement via diffusion during shear-band cooling. This model is referred to as *Progressive Subgrain Misorientation* recrystallization and appears to account for shear band microstructures in a variety of metals.

- "FLOW STRESS OF FCC POLYCRYSTALS WITH APPLICATION TO OFHC CU" S. Nemat-Nasser and Y. Li.

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Abstract

Based on the concept of dislocation kinematics, paralleled with a systematic experimental investigation, a physically-based model is developed for fcc polycrystals, using OFHC copper for illustration. First, the concept of the motion of dislocations and the barriers that they must overcome in their motion, is used as an underlying motivation to obtain general expressions which include a number of free constitutive parameters. These parameters are then evaluated by direct comparison with experimental data. High-strain-rate compression experiments are performed using the UCSD's recovery Hopkinson technique: see Nemat-Nasser *et al.* (1991, 1994), and Nemat-Nasser and Isaacs (1996). Strains close to 100% are achieved in these tests, over a temperature range of 77 to 1,100K, and strain rates of 10^{-3} to 8,000/s; the quasi-static tests are performed using an Instron machine. For low-temperature tests, both the as-received and annealed samples are tested. Good correlation between the theoretical predictions and experimental results (especially at high stain rates) is obtained with few free constitutive parameters. The orders of magnitude of several of these parameters are first estimated based on the underlying structure of the material. Experimental results are then used to tune the final values of these parameters. It turns out that the structure of the constitutive relations and the value of a number of the constitutive parameters are essentially the same for commercially pure tantalum (bcc metal) and OFHC copper. The relation between the two cases is examined and the similarities and differences are discussed.

Work in Progress - Selected Papers

- "A PHYSICALLY-BASED CONSTITUTIVE MODEL FOR BCC CRYSTALS WITH APPLICATION TO POLYCRYSTALLINE TANTALUM" S. Nemat-Nasser, T. Okinaka and L. Ni

Abstract

Based on the results of an extensive series of systematic experiments on commercially pure tantalum (bcc crystals), a physically-based, rate- and temperature-dependent constitutive model is proposed for bcc single crystals and is applied to simulate the experimental results, using the Taylor averaging method. The model calculation is based on a new, efficient algorithm for the solution of finite-deformation of bcc single crystal, involving up to forty-eight potentially active slip systems. The accuracy and efficiency of the proposed algorithm are checked through comparison with the results of the conventional explicit Euler time-integration scheme, using a very large number of timesteps. The model effectively simulates a large body of experimental data, over a broad range of strain rates (10^{-3} to 4×10^4/s,) and temperatures (77 to 1300K), and strains exceeding 100%, using very few adjustable parameters which, however, are fixed for a given material. All other involved constitutive parameters are estimated based on the crystal structure and the physics of plastic flow.

- "MICROSTRUCTURE OF HIGH-STRAIN-RATE DEFORMED TANTALUM"
  S. Nemat-Nasser, J.B. Isaacs and M. Liu

Abstract

Hat-shaped specimens of polycrystalline tantalum are subjected to high plastic shear strains ($\gamma = 170$ to 910%) at strain rates exceeding 5×10^4/s in a compression split Hopkinson bar. The dynamic shear tests are performed at room and 600K initial temperatures, under adiabatic and quasi-isothernal conditions, using UCSD's recovery Hopkinson technique. The microstructure of the post-test specimens is examined with transmission electron microscopy (TEM). The plastic deformation is highly concentrated, producing a narrow shear-localization region of approximately 200μm in width. Slip of perfect screw dislocations, on the {110} primary planes along the <111> directions, is found to be the dominant deformation mechanism. Dynamic recovery takes place in the shear-localization regions of all adiabatically tested specimens, and evidence of dynamic recrystallization is observed in the

specimen deformed to a shear strain of 910% at a 600K initial temperature. The substructures of the adiabatically tested specimens include well-defined dislocation arrays, grouped dislocations, elongated dislocation cells, subgrains, and recrystallized micro-sized grains. The microstructure of isothermally tested specimens, on the other hand, features high dislocation density and inhomogeneous dislocation distribution. In light of the TEM observations, the relationship between the microstructure and shear stress, the caused of strain inhomogeneity, the estimated adiabatic temperature within the shear-localization zone, the rapid quenching of the shearband at the end of the dynamic testing, the slip characteristics of dislocations in tantalum, and the formation mechanisms of dislocation loops, are discussed.

- "DYNAMIC FLOW LOCALIZATION IN FCC SINGLE CRYSTALS" by S. Nemat-Nasser, T. Okinaka, V. Nesterenko and M. Liu

Abstract

Localization of the inelastic flow and crack initiation in fcc single crystals are studied experimentally and by numerical simulations, focusing on the anisotropic inelastic response of the crystal, and the mechanisms of possible crack initiation and growth, produced upon unloading by the residual inhomogeneous plastic strains. Hollow circular cylinders of single-copper are subjected to externally applied explosive loads which cause the collapse of the cylinder; this procedure is called the thick-walled cylinder (TWC) method. Then, numerical simulations are performed to understand the deformation process which leads to localized deformation, and tensile cracking when partial collapse is followed by unloading. Various loads and initial orientations of the lattice are examined in these numerical simulations in order to study their effects on the flow localization and crack initiation phenomena.

LISTING OF PUBLICATIONS SUPPORTED UNDER THIS GRANT

PUBLICATIONS

The following manuscripts, submitted for publication, in press, and published, were prepared wholly or partially under the sponsorship of the Army Research Office, DAAL03-92-G-0108.

A. Published Manuscripts

1. "Crystal Plasticity," Nemat-Nasser, S. and A. Agah-Tehrani, *Proceedings of ASME-WAM,Symposium on Defects and Inelasticity in the Characterization of Crystalline Solids*, L.M. Brock (ed.), AMD-Vol. 148, Book #G00746 (1992).

2. "A New Finite-Deformation Constitutive Algorithm and Its Finite-Element Simulations of The Controlled Adiabatic Shear Banding," Nemat-Nasser, S., and Y.-F. Li, Proceedings of the 2nd International Conference on Discrete Element Methods (DEM), at IESL, MIT, Cambridge, MA, March 18-19, 1993, *Theory of Application,* J.R. Williams and G.G.W. Mustoe (eds.) (1993), 425-436.

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3. "Experimental Evaluation of Strain, Strain-Rates, and Temperature Dependence of Flow Stress at High Strain Rate," Nemat-Nasser, S., Y.-F. Li, and J.B. Isaacs, Proceedings of MEET'N'93,the 1st Joint Meeting of ASCE, ASME, and SES, *Experimental Techniques in the Dynamics of Deformable Solids*, University of Virginia, Charlottesville, VA, June 6-9, 1993, AMD-Vol. 165 (1993), 25-32.

4. "An Explicit Integration Scheme for Finite-Deformation Plasticity in Finite-Element Methods," Li, Y.-F. and S. Nemat-Nasser, *Finite Elements in Analysis and Design*, Vol. 15 (1993), 93-102.

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8. "Experimental/Computational Evaluation of Flow Stress at High Strain Rates with Application to Adiabatic Shear Banding," Nemat-Nasser, S., Y.-F. Li and J.B. Isaacs, at the SES Conference at UCSD, September 1992, special issue of *Mechanics of Materials*, Vol. 17 (1994), 111-134.

9. "An Algorithm for Large-Scale Computational Finite-Deformation Plasticity," Nemat-Nasser, S. and Y.-F. Li, *Mechanics of Materials*, Vol. 18 (1994), 231-264.

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11. "Evolution of Microstructure and Shear-Band Formation in α -hcp Titanium," Meyers, M.A, G,. Subhash, B. Kad and L. Prasad, *Mech of Matls,* Vol. 17 (1994), 175-193. (acknowledges Army Research Office).

12. "Dynamic Failure: Mechanical and Microstructural Aspects," Meyers, M.A., Proc. EURODYMAT 94, *J. de Physique III*, ed. J. Harding, Vol. 4, (1994) C8-597-621. (acknowledges ARO URI Program).

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15. "Effects of Shock Loading on Cobalt-Based Solid-Solution Strengthened Superalloys," Vecchio, K.S. and A.M. Thakur, *Journal de Physique IV, Colloque C8*, supplement au Journal de Physique III, Vol. 4, (1994), 367-372.

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"High-Strain, High-Strain-Rate Response of Annealed and Shocked Tantalum", LaSalvia, J.C., Y.J. Chen, M.A. Meyers, Y.F. Nesterenko, M.P. Bondar and Y.L. Lukyanov, *Tantalum, TMS-AIME*, Warendale, PA. in press (1996). (also supported by ARO DAAH-04-93-G-0261 to the University of California, San Diego).

"Investigation of High-Strain, High-Strain-Rate Behavior of Tantalum Using the Collapse of a Thick-Walled Cylinder," Nesterenko,V.F., M.A. Meyers, J.C. LaSalvia, M.P. Bondar, Y.J. Chen, and Y.L. Lukyanov, *Matls. Sci. And Eng.*, in press (1997).

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"Deformation Behavior of Tantalum and a Tantalum Tungsten Alloy," R. Kapoor and S. Nemat-Nasser, *Proceedings of Symposium Advances in Inelastic Flow and Fracture*, SES 1998, Pullman, Washington, accepted 9/98. ARO DAAL 03-92-G-0108 to UCSD.

C. Manuscripts Submitted

"Self-Organization in the Initiation of Adiabatic Shear Bands" Meyers, M.A., V. Nesterenko and T. Wright, *Acta Met. et. Mat.*, submitted 1997. (also supported by ARO DAAH-04-94G0314 to UCSD, Naval Research and the U.S. Army Research Laboratory).

"Effect of Stain Rate on Plastic Flow and Failure in Polycrystalline Tungsten," Dummer, T., J.C. LaSalvia, G. Ravichandran, and M.A. Meyers, *Acta Materialia,* submitted 1996.

D. Work in Progress

Book:

Plasticity: A Treatise on Finite Deformation of Heterogeneous Inelastic Solids, by Nemat-Nasser, S. Approx. 700 pages, in preparation.

E. Related Publications Supported by Other Contracts and Grants

"Constitutive Description of Work- and Shock -Hardened Copper," Andrade, U., M.A. Meyers, and A.H. Chokshi, *Scripta Met. et. Mat*, Vol 30 (1994) 933-938. (acknowledges ARO DAAL-03-86-K-0167 and MSS 90-2167 to UCSD).

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"Dynamic Recrystallization and Grain Size Effects in Shock-Hardened Copper," Andrade, U., M. A. Meyers, A. H. Chokshi, and K. S. Vecchio, *Journal de Physique IV, Colloque C8*, supplément au Journal de Physique III, Vol. 4, (1994), 361-366. [Acknowledges ARO DAAL03-86-K-0169 to UCSD and NSF MSS-9021671 to UCSD].

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"Tantalum Microstrucrures for High-Strain-Rate Deformation: Shock Loading, Shaped Charges, and Explosively Formed Penetrators," Murr, L.E., S. Pappu, C. Kennedy, C-S Niou, and M.A. Meyers, *Tantalum, TMS-AIME*, to be published 1996. (acknowledges U.S. Army ARDEC DAAA-21-94-C-0059 to the University of Texas, El Paso).

"Deformation Twins in a Shock-Loaded Ta-2.5^{w}/o W Precursor Plate and a Receovered, Ta-2.5^{w}/oW Explosively Formed Penetrator." Pappu, S., C. Kennedy, L.E. Murr and M.A. Meyers, *Scripta Mat,* to be published (1996). (acknowledges U.S. Army ARDEC DAAA21-94-C-0059 to the University of Texas, El Paso).

"Collective Behavior of Shear Bands," Nesterenko, V.F., M.A. Meyers and T.W. Wright, *Metallurgical and Materials Applications of Shock-Wave and High-Strain-Rate Phenomena*, eds. L.E. Murr, K.P. Staudhammer and M.A. Meyers, Elsevier, (1996) 397-404 (Supported by ARO DAAH-04-94G0314 to UCSD and Office of Naval Research, Contract N00014-94-1-1040 and by the US Army Research Laboratory).

"Effects of Interstitials on the Mechanical Behavior of Tantalum," Strutt, A., K.S. Vecchio, S.R. Bingert, and G.T. Gray, III, *Proceedings of the International Conference on Tungsten and Refractory Metals*, (1996). (acknowledges work sponsored through LANL as part of the DoD/DOE Joint Office of Munitions Project on High Density Materials).

SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED

Scientific Personnel:
Abbas Azhdari (7/95-1997 - partially supported), Postdoctoral Researcher. Research focused on implementation of a new integration routine for constitutive equations into the FEM codes dyna2d and dyna3d; improving the accuracy and efficiency of the currently used computational routines is the goal. *PI: S. Nemat-Nasser*

Masoud Beizaie (7/95 to 1997 - partially supported) Assistant Research Engineer. Research focused on development of theoretical models for the dynamic behavior of pure tantalum and tantalum-tungsten alloys in a wide range of strain rates and temperatures. *PI: S. Nemat-Nasser*

Mingqui Liu (9/95 to 11/20/97- partially supported) Postdoctoral Researcher. Research focusing on microstructural characterization at nano-scale of dislocation structure within an adiabatic shearband with accumulated shear strains from a few hundred too greater than 900%. The relation between dislocation structure, the induced temperature exclusion, and dynamic re-crystallization is examined in detail and many interesting facets are revealed. *PI: S. Nemat-Nasser*

Luqun Ni (3/93 to 1997 – partially supported) Assistant Research Engineer. Research focused on the areas of dynamic interface cracks. *PI: S. Nemat-Nasser*

Andrew Strutt (7/1/95-1997 - work supported through Los Alamos National Lab). Research on the role of interstitials in powder metallurgy processed tantalum alloys. *PI: K. Vecchio*

Graduate Research Assistants:

Y.C. Chen (1/95-present) (partially supported), research focusing on high strain, high strain rate behavior of tantalum and shock loading effects. *PI: M.A. Meyers*

Rajeev Kapoor (10/95 - 1997), research focused on work in the area of high strain rate deformation of Al-based metal-matrix composites *Ph.D.* Degree Awarded Summer 1998, Title of Dissertation: "Deformation Mechanisms During Compressive Loading of Tantalum and tantalum-2.5 Weight % Tungsten". . *PI: S. Nemat-Nasser.*

Tomoo Okinaka (9/95 – 10/96), research focused on finite deformation of single crystals which have a face centered cubic structure. Particularly, a flow localization and cracking of single crystals due to their anisotropic inelastic response is studied both experimentally and numerically. Ph.D. Awarded Fall 1996. Title of Dissertation: "Finite Deformation of FCC Single Crystals: New Computational Approach to Flow Localization Phenomena". *PI: S. Nemat-Nasser.*

Sanwu Tan (8/95 - 6/96), research focused on a new algorithm for Johnson-Cook model in DYNA3d, implementation of generalized radial-return method, and plasticity models for granular materials. *PI: S. Nemat-Nasser.* [Effective Fall 1996, Mr. Tan is now a graduate student with UCSD's CMRR]

Aashish Rohatgi (9/93 to present), research focusing on the investigation of the deformation behavior of Cu and Cu-Al alloys and to study the role of SFE. *PI: K.S. Vecchio*

REPORT OF INVENTIONS (BY TITLE ONLY): NONE

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INTERACTION WITH DOD, DOE LABORATORIES, INDUSTRY, AND UNIVERSITIES

The UCSD team has had extensive collaborative interaction with DoD, DOE, and a number of other institutions, including universities and particularly ARL, over the past year. Some of these are summarized below.

ARL

- **Dr. Thomas W. Wright** visited CEAM on the program focusing on collective behavior of shearbands, as well as a research program on analytical modeling of adiabatic shearbands. The current work has led to two papers, co-authored with Dr. Meyers, entitled "Collective Behavior of Shear Bands," and "Self-Organization of Shear Bands in High-Strain-Rate Deformation", as well as to a paper under development with Professor Nemat-Nasser and Dr. Luqun Ni., on "Asymptotic Solution of an Advancing Adiabatic Shearband".

- **Dr. Shun-Chin Chou** and **Dr. Tusit Weersooriya**: CEAM has developed a state-of-the-art combined tension/compression recovery Hopkinson bar which has been constructed at UCSD. We expect that Dr. Weersooriya will visit UCSD and will receive advice on the use of the instrument and then the instrument will be transferred to ARL. We expect to have continued interaction with Drs. Chou, Weersooriya, and Dandekar on high-strain-rate property measurements based on this novel recovery Hopkinson bar system.

- **Dr. Lee Magness** is interacting with Dr. Nemat-Nasser and coworkers on developing effective tungsten-based composite alloys.

- Dr. Asaro and his coworkers have continued interaction with **Dr. Scott Schoenfeld**, former graduate student at UCSD and now a project scientist at ARL.

ARDEC

- CEAM is interacting with **Drs W. Ebihara** and **D. Kapoor** in developing test techniques based on the hat-shaped specimen to screen materials for their dynamic properties and particularly their propensity toward adiabatic shearbanding.

Naval Surface Warfare Center

- CEAM interacted with **Mr. Leonard Wilson** in developing a state-of-the-art combined tension/compression recovery Hopkinson bar system, based on CEAM's novel techniques. This interaction included teaching the use of the system and training Navy personnel.

DOE

Lawrence Livermore National Lab

- Professor Meyers has collaborated with **Dr. D. Lassila** on a program focusing on high-strain, high-strain rate response of shocked tantalum. As a joint venture, the LLNL and UCSD specimens were shock hardened at New Mexico Tech using an explosive set-up with an impact velocity of ~ 1,300m/s. Shocked samples have been tested at CEAM of UCSD and are now being analyzed.

- The UCSD group is closely interacting with **Dr. W. Nellis**, who is in charge of the gas gun facility at LLNL.

Los Alamos National Lab

- Dr. George T. Gray has been interacting with Professor K. Vecchio on research focusing on the dynamic behavior of tantalum, tantalum/tungsten, and tungsten-based and other composites. Several papers have been completed; "Shock-Loading Response of 6061-T6 Aluminum-Alumina Metal-Matrix Composites," "Effects of Shock Loading on a Solid-Solution Strengthened Supper Alloy," and "Influence of Peak Pressure and Temperature on the Structure/Property Response of Shock-Loaded Ta and Ta-10W".

- Professor Vecchio's project on the development of a new tungsten heavy alloy which uses the HAYNES 230 alloy at the binder phase, involved collaboration with **S. Bingert, H. Sheinberg,** and **P. Dunn** of the Solidification Technology group. This interaction is focused on developing several different processing routes for fabrication of a large-scale sample.

- Professor Nemat-Nasser has been interacting with **Drs. A. Rollett, J.D. Cotton, George T. Gray,** and **Mr. R. Rhorer** on developing tantalum-titanium alloys with special high-temperature properties.

- **Dr. Shihong Gary Song**, formally at LANL, is now doing microscopy on tantalum samples which have been tested at CEAM. This work is in collaboration with Professor Nemat-Nasser and his coworkers.

UNIVERSITY & INDUSTRY

- CEAM has been working very closely with two historically black universities: **Prairie View A&M University** (PVAMU) and **Tuskegee University (TU)**. **Dr. J. Zhou** and **Dr. Dean Baker** at PVAMU and **Professors S. Jeelani** and **H. Mahfuz** at Tuskegee University are the collaborating faculty members. CEAM has built an 11/2 inch Hopkinson bar for TU and has instructed scientists at TU on how to use this instrument. CEAM is now in the process of constructing a 3inch gas gun for TU.

- CEAM is providing support for an ARO project, entitled "Intelligent Resin Transfer Molding for Integral Armor Applications". **Tuskegee University (TU)** is the lead institution, with the University of Delaware's Center for Composite Materials, North Carolina A&T State University's Center of Excellence for Electronics and Communication, PVAMU, and UCSD's CEAM and the Institute for Mechanics and Materials (IMM) as team members. This is a five-year project working on developing high-performance composites and composite hybrids for the Composite Armored Vehicle (CAV) for the Army.

  Current interactions included a visit by Dr. Anwar Haque (Tuskegee University), whereby he was instructed on the use, maintenance and repair of strain gauges; Ms. Roshan Raines, a graduate student from Tuskegee University, who performed a 3- month summer internship at CEAM on research focusing on the testing of S2 glass fiber composite materials; and Ms. Atieno Obala, a

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undergraduate student from Prairie View, A&M, who performed a 3-month summer internship at CEAM, observing research testing on cylindrical shaped Ta-2.5%W and Al-Li materials.

- Professor Meyers' program on high-strain, high-strain rate response involves thick-walled cylinder-collapse experiments on unshocked and shocked specimens. The cylinder-collapse tests were carried out in collaboration with **Professor V.F. Nesterenko,** at the Institute of Hydrodynamics in Russia; four cylinder-collapse experiments were carried out. Professor Nesterenko's collaborators at the Institute of Hydrodynamics are M.P. Bordav and Y.L. Lukyanov. (Note: In March 1996, Professor Nesterenko was appointed as an Associate Professor-in-Residence, UCSD Department of Applied Mechanics and Engineering Sciences).

- The metallographic characterization (primarily TEM) of the shocked tantalum is being carried out by **Professor L.E. Murr** and co-workers at the **University of Texas at El Paso (UTEP).** The UCSD graduate student working on this program, Mr. Y. -J. Chen, visited UTEP and participated in all stages of characterization. **Dr. J.C. La Salvia**, Post-Doctoral Researcher at UCSD's IMM, took an active part in the analysis of the material.

- Graduate student Mr. Tomoo Okinaka has used crystal plasticity models and the new algorithm of Professor Nemat-Nasser to model the process of collapse of single crystal thick-walled copper cylinder. The experiment has been performed in collaboration with **Professor Nesterenko.**

- Professor Meyers' program on dynamic behavior of polycrystalline tungsten involved collaboration with **Mr. Tobias Dummer**, a visiting student from the **University of Karlsruhe, Germany**.

- CEAM has developed a special testing device to measure the flow stress of very thin film (about 100mm thickness) for **Honeywell,** and has successfully measured the stress-strain relations for specimens which were provided (these specimens were about 100mm by 1mm by 2mm size).

- CEAM interacted with **CERCOM Inc.** on a number of projects relating to hybrid composites for lightweight armor.

- Professor Vecchio's program on Computational Banding in Ta-10W Alloys, and the Role of Interstitials in Powder Metallurgy Processed Tantalum Alloys, involved interaction with **Cabot Corporation**, who provided materials for this research program.