

REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-04-

0487

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for review the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or reducing this burden to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson (Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE 09/07/2004		3. REPORT TYPE AND DATES COVERED Final report	
4. TITLE AND SUBTITLE ADVANCED COMPUTATIONAL TECHNIQUES FOR THE DESIGN OF DEFORMATION PROCESSES				5. FUNDING NUMBERS AFOSR CONTRACT NO. F49620-00-1-0373	
6. AUTHOR(S) Prof. Nicholas Zabaraz. Materials Process Design and Control Laboratory, 188 Rhodes Hall, Cornell University, Ithaca, NY 14853-3801					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Cornell University Office of Sponsored Programs 120 Day Hall Ithaca, NY 14853				8. PERFORMING ORGANIZATION REPORT NUMBER OSP 38032	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR, Computational Mathematics program, 4015 Wilson Blvd, Room 817-A Arlington, VA 22203-1954 (Dr. F. Fahroo program manager, (703) 696-8429, fariba.fahroo@afosr.af.mil)				10. SPONSORING / MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES					
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release, distribution unlimited				12b. DISTRIBUTION CODE Approved for public release, distribution unlimited	
13. ABSTRACT (Maximum 200 Words) The objective of this work is to develop a continuum sensitivity finite element analysis for the robust design of multi-stage metal forming processes in aircraft manufacturing. The computational forming design simulator being developed is applied to industrial forming design and provides the means to select the sequence of deformation processes, design the dies and preforms for each process stage as well as the process conditions such that a product is obtained with desired shape and microstructure and with the minimum material utilization and overall cost. The initial selection of the various processing stages are done a-priori and through the use of classification schemes operating on a digital materials and process library. This virtual process laboratory will assist the aircraft manufacturing industry in reducing time for process and product development, in trimming the cost of an extensive experimental process development effort and in developing processes for tailored material properties.					
14. SUBJECT TERMS				15. NUMBER OF PAGES	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT		18. SECURITY CLASSIFICATION OF THIS PAGE		19. SECURITY CLASSIFICATION OF ABSTRACT	
				20. LIMITATION OF ABSTRACT	

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

BEST AVAILABLE COPY

20040930 017

ADVANCED COMPUTATIONAL TECHNIQUES FOR THE DESIGN OF DEFORMATION PROCESSES

FINAL REPORT: AFOSR CONTRACT NO. F49620-00-1-0373

PI: Prof. Nicholas Zabaras

Materials Process Design and Control Laboratory, Sibley School of Mechanical and
Aerospace Engineering, Cornell University, 188 Frank H.T. Rhodes Hall, Ithaca,
NY, 14853-3801, USA. E-mail: zabaras@cornell.edu
URL: <http://www.mae.cornell.edu/zabaras/>

Summary of project objectives and accomplishments

The objective of this project was to develop a continuum sensitivity finite element analysis for the robust design of multi-stage metal forming processes in aircraft manufacturing. The computational forming design simulator being developed was applied to several industrial forming design applications. It provides the means to select the sequence of deformation processes, design the dies and preforms for each process stage as well as the process conditions such that a product is obtained with desired shape and microstructure and with the minimum material utilization and overall cost. The initial selection of the various processing stages are done a-priori and through the use of classification schemes operating on a digital materials and process library. This virtual process laboratory will assist the aircraft manufacturing industry in reducing time for process and product development, in trimming the cost of an extensive experimental process development effort and in developing processes for tailored material properties.

1 Review of project accomplishments

The high cost of manufacturing critical structural components can be greatly reduced with the development of mathematically and physically sound computational methodologies for process design and control. Metal forming design, therefore, requires an accurate description of the thermo-mechanical deformation mechanisms in order to simultaneously achieve two or more design objectives defined in Box 1. Such design objectives are subject to processing constraints like maximum press capacity, zone of processing temperatures, final product quality and cost. These objectives can be achieved by proper design of the initial shape of the workpiece, the shape of the die, the ram speed, the initial state of the workpiece and die and other process parameters. The complexity of metal forming design is apparent considering the number of coupled non-linear physical mechanisms that need to be accounted for, such as (a) large deformation polycrystal plasticity, (b) deformation induced microstructure evolution, (c) time varying contact and friction conditions, (d) thermal effects and mechanical dissipation and (e) damage accumulation leading to material rupture. The role of these mechanisms in the processing of the initial workpiece to yield the final product is paramount and in almost all cases of design, intermediate processing stages need to be

DISTRIBUTION STATEMENT A
Approved for Public Release
Distribution Unlimited

used to efficiently transform the initial geometry/material into the desired final shape and material properties.

A number of significant contributions have been made, over the last 4 years, in the development of a virtual materials and process design simulator. In particular:

- A computational sensitivity framework was developed to evaluate the shape and parameter sensitivities of finite coupled thermo-inelastic deformations using the continuum sensitivity method (CSM) [1]-[4].
- Continuum sensitivity method was developed for large thermo-plastic deformations combined with ductile damage. This sensitivity framework is used for the design of metal forming processes of porous materials [5].
- A mathematically rigorous CSM was implemented for the design optimization of multi-stage deformation processes. This multi-stage analysis takes the form similar to an updated Lagrangian framework for the design of single-stage processes. It also allows us to treat shape and parameter sensitivities in a unified manner [6].

- Minimization of material usage
- Uniform deformation in the final product
- Minimum required work or forming force
- Desired microstructure in the final product
- Minimum or desired residual stress distribution
- Minimum deformation and wear of the die
- Desired shape of the final product
- Minimum porosity in the final product

Box 1: Objectives in hot forming design that have been integrated in the virtual design environment developed under this AFOSR project.

- A framework was developed for modeling of dynamic recrystallization and related grain growth processes by explicitly incorporating the various microstructural length scales that describe the state of the evolving microstructure. In addition, a methodology was developed [7] for the control of mean grain size during thermo-mechanical deformation processes. The main reason for this renewed interest lies in the attractiveness of control of microstructural properties in metallic materials by thermomechanical processing rather than by alloying - the current, expensive industrial practice.
- The design simulator was extended towards the design of polycrystalline materials. This is critical as most airframe and engine applications use materials that are polycrystalline in nature. The properties of these materials depend not only on the properties of the individual crystals but also on parameters, like the crystallographic orientation (texture), that characterize the polycrystal. This texture further characterizes

the mechanical, thermal and magnetic behavior of the material. In particular, several design problems of industrial interest are addressed in [8, 9]. Further, this polycrystalline model was extended to incorporate thermal and mechanical processing effects on texture [10].

- In conjunction with polycrystalline plasticity, a classification methodology [11, 12] was developed which has helped develop and maintain a digital materials and process library. Further, the classification tool has led to an effective selection of processing stages eliminating the need for expert knowledge.
- In addition, the present virtual design simulator was extended towards modeling and design of 3D processes and involved the development of novel algorithms for handling contact and friction problems at the die workpiece interface in both the direct and sensitivity problems. As part of developing solutions for complex industrial problems, remeshing and data transfer issues were addressed [13, 14].

The developed forming design simulator can address a variety of design problems for geometrically complex two-dimensional, axisymmetric and three-dimensional multi-stage deformation processes. Such intermediate processing stages help the designer by introducing more flexibility in the design process. The developed design simulator is mathematically and computationally rigorous, and is based on a gradient-based optimization methodology. The virtual materials process design simulator is based on quantified product quality and accounts for process targets and constraints. This simulator depicted in Box 2 includes the development of a continuum sensitivity analysis consistent with the virtual direct process simulator and is capable of accurately computing the gradients of objective functions and process constraints.

- 1. Mathematical representation of the design objective
- 2. Selection of the sequence of processes (stages) and initial process parameter designs using knowledge based expert systems, microstructure evolution paths and/or ideal forming techniques
- 3. Selection of the design variables (e.g. parametric representation of dies/preforms)
- 4. Selection of a virtual direct process model
- 5. Interactive optimization environment
- 6. Continuum multi-stage process sensitivity analysis consistent with the direct process model
- 7. Optimization algorithms
- 8. Assessment of automatic process optimization

Box 2: A computational design simulator for forming processes.

The advantages of such a design simulator are substantial and are discussed as needed. In the next few sections, particular achievements of this project are briefly described. For more

details, the original comprehensive references that discuss these developments in detail can be downloaded from our laboratory's web site.

1.1 The CSM for hot-forming design [4]

A computational framework has been developed to evaluate the shape as well as non-shape (parameter) sensitivity of finite thermo-inelastic deformations using the continuum sensitivity method (CSM). Weak sensitivity equations are developed for the large thermo-mechanical deformation of hyperelastic thermo-viscoplastic materials that are consistent with the kinematic, constitutive, contact and thermal analyses used in the solution of the direct deformation problem. The sensitivities are defined in a rigorous sense and the sensitivity analysis is performed in an infinite-dimensional continuum framework. The effects of perturbation in the preform, die surface, or other process parameters are carefully considered in the CSM development for the computation of the die temperature sensitivity fields. The direct deformation and sensitivity deformation problems are solved using the finite element method. The results of the continuum sensitivity analysis are validated extensively by a comparison with those obtained by finite difference approximations (i.e. using the solution of a deformation problem with perturbed design variables). The effectiveness of the method has been demonstrated with a number of applications in the design optimization of metal forming processes.

One representative example involved the preform design for closed-die forging process. Most industrial design problems involve multiple objectives and an attempt is made to discuss such design issues in this example. It concerns the estimation of the volume of the preform as well as the design of the free surface of the preform so as to completely fill a given die cavity with minimum flash and result in a product with uniform scalar state variable (deformation resistance parameter). A non-isothermal die with an initial temperature of 473 K is used. The die is described in [4]. The free surface $R_{\beta}(\alpha)$ is represented as a degree 6 Bézier surface. The reference preform was chosen as a right circular cylinder whose volume was nearly equal to the volume enclosed by the die cavity. The initial preform used was of dimensions 0.7 mm (radius) \times 1.2 mm (height) and it was of less volume than the die cavity. The simulation parameters used in this example are tabulated in [4]. The distributions of the state variable in the product obtained using the initial preform, the optimal preform and the reference preform discussed above are given in Figure 1. Further, Figure 2 provides the optimum preform shape. The computed average values of the state variable in the product obtained using the reference and optimal preforms are given as 40.8 MPa and 40.0 MPa, respectively. To quantify the extent of reduction in the variation of the state variable, we also evaluated the average deviation of the state variable in the obtained products. It is given as 1.819 MPa for the product obtained using the reference preform and 1.174 MPa for the product obtained using the optimum preform.

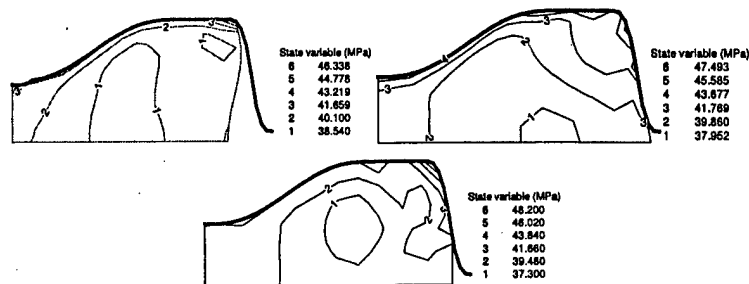


Figure 1: Comparison of the state in the final product using initial, optimal and reference preforms.

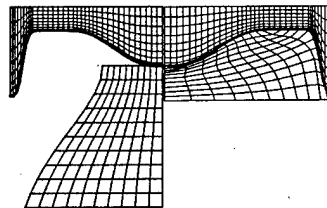


Figure 2: Optimal preform shape needed to fill the die and minimize the deviation in state variable in the final product.

1.2 The CSM for materials with ductile damage [5]

A continuum sensitivity method has been developed for thermoplasticity combined with ductile damage at finite strains [5]. The computed sensitivity fields are used within a gradient-based optimization framework for the computational design of metal forming processes for porous materials. The accuracy and effectiveness of the developed updated Lagrangian finite element analysis and design techniques were demonstrated with a number of representative examples. In addition to die design problems, novel preform (shape) design problems were examined for near net shape manufacturing that accounts for the volume change induced during the deformation process. In particular, the volume void fraction is taken to be the damage parameter, whose evolution equation is obtained from the conservation of mass of the matrix material. In addition, the body is assumed to behave as a continuum despite the presence of microvoids.

An example of the applicability of the design simulator is discussed next. The objective here is to design the volume and the free surface of a cylindrical preform of height 2.0 mm, that when compressed with a given closed forging die, fills the die completely with minimum or no flash, after a specified stroke of 0.65 mm. The workpiece material is taken to be Fe-2%Si with a 5% porosity, at an initial temperature of 1273 K. The desired final radius around the flash is taken as 1.2 mm and the desired height at $r = 0$ as 0.7 mm. The particular die for this problem is defined in [5]. Since the problem is complex in nature, it involves multiple

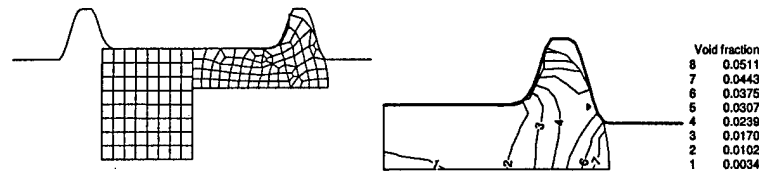


Figure 3: Initial guess preform shape, the final product using this guess and the distribution of void fraction in the final product for a thermomechanical closed die forging process. For a non-porous material, this preform will fill the die as required without flash.

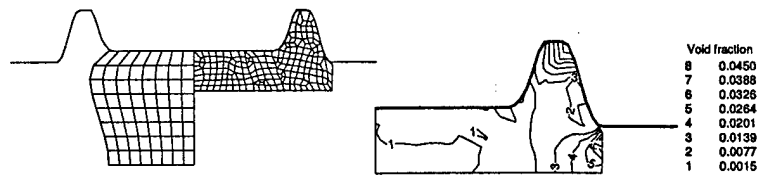


Figure 4: Optimal preform shape, the final product using this preform and the distribution of the void fraction for a thermomechanical closed die forging process.

remeshing operations. The free surface $R_{\beta}(\alpha)$ is represented with a degree 6 Bézier curve as in the first example. Figure 3 shows the quarter geometry of the initial guess preform (a right circular cylinder of radius 0.8 mm and height of 2 mm). Also shown is the final product shape obtained using this reference preform. Figure 4 shows the optimal preform and the final product shape achieved using this optimal preform.

1.3 Design of multi-stage material processing operations [6]

A novel, efficient and mathematically rigorous continuum based sensitivity method has been developed which can be used to accurately evaluate the gradients of the objective function and constraints in the optimization-based design of multi-stage deformation processes. Weak sensitivity equilibrium equations are derived for the large deformation of the workpiece in each forming operation. This sensitivity kinematic problem is linearly coupled with the corresponding continuum sensitivity constitutive, contact and thermal sub-problems for the particular process. Thus a linear sensitivity problem with appropriate driving forces is identified and the analysis is carried out in an infinite dimensional framework. The multi-stage continuum sensitivity analysis takes a form similar to the updated Lagrangian sensitivity framework developed earlier for the design of single-stage deformation processes. It allows us to treat in a unified manner shape and parameter sensitivity analysis that are both present in a typical design problem of multi-stage deformation processes. The effectiveness of the proposed methodology is demonstrated with the solution of

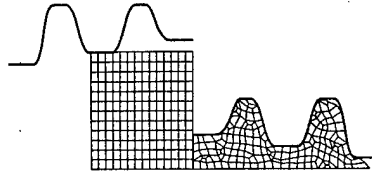


Figure 5: Reference one-stage design using a right-circular cylinder of the required volume.

three practical problems in the design of two-stage metal forming processes.

We present an example involving forging process design for producing an (axisymmetric) ribbed disk. The initial billet is a right cylinder of 2 mm height and 0.88 mm radius. The height reduction at $r = 0$, in the first stage is 0.9 mm and in the second stage is 0.5 mm. A quarter of the billet is modelled in the simulation and design. For simplicity of the design process, isothermal process conditions (673 K) are assumed herein. The finishing die geometry is defined in [6]. When a single stage process is considered (using a right-circular cylinder of the fixed required volume of 4.93 mm^3), one can notice from Figure 5 that the die cavity cannot be filled in the upper-right corner. To overcome this problem, a possible solution will be to start with considerably more material than that required. However, this could lead to a high forging force and sizeable increase in flash. An alternative solution to this problem is to design a multi-stage process, in which the initial billet (right circular cylinder) is preformed to some intermediate shape. This preform is then formed to the desired shape using the finishing die. The solution reported has demonstrated that the design intent of the final product can be achieved with a two-stage process. The design example is thus re-posed as a two-stage design problem, where an open die is adopted in the performing stage and a closed die in the finishing stage. In the design process, the closed die is kept unchanged to form the desired boundary of the final product and the objective is to design the open die shape such that the finishing die cavity can be completely filled. Figure 6 shows the design process of the performing die. When an initial guess (flat die) is used, a noticeable gap appears at the top of the outer cavity, where as the design preforming die shape results in completely filling the cavity. Finally, a comparison of the force histories for the reference (non-optimized) one-stage design process and the two-stage optimal process computed using the CSM method is provided in Figure 7. Even though, the objective of the simulation was to solely control the shape in the final product, it is apparent that, as byproduct of the design simulation, a reduction in the maximum force was obtained as well.

1.4 Design of materials undergoing dynamic recrystallization [7]

The idea of control of mechanical properties in materials through designer processing techniques is promoted through this effort, in contrast to the standard control by alloying. Microstructure evolution through dynamic recrystallization is accurately modelled for the large thermo-mechanical deformation of hyperelastic thermo-viscoplastic materials. An in-

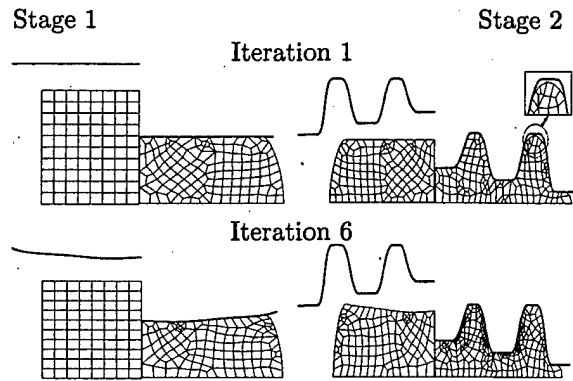


Figure 6: Comparison of the final product obtained using the initial and optimal solution for the thermo-mechanical preform forging design problem.

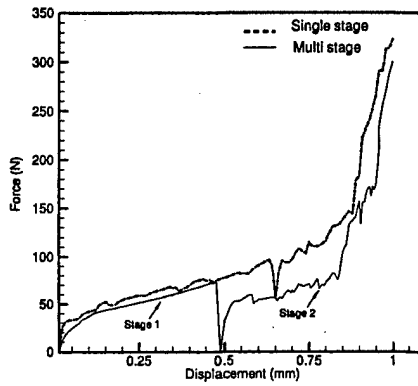
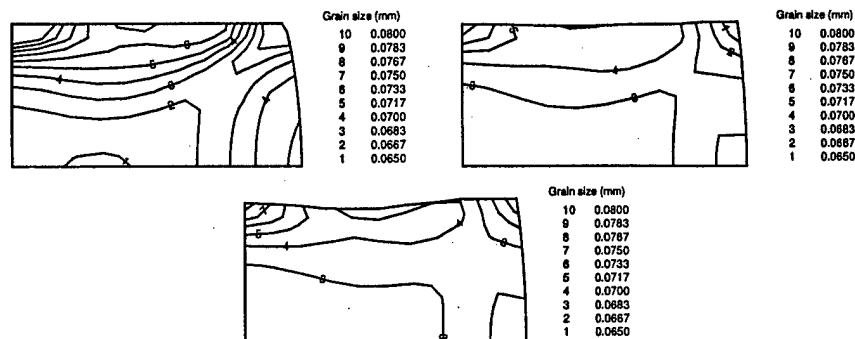


Figure 7: A comparison of the required forging force histories for the one-stage reference design and the two-stage optimal design.



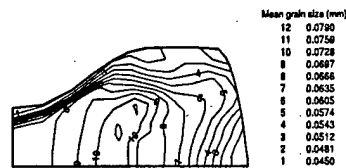
(c) Optimum design iteration

Figure 8: Variation of the mean grain sizes and the intermediate preform using various die shapes during the optimization process.

novative solution strategy and a computational algorithm are developed for the solution of the direct deformation problem comprised of the kinematic, constitutive, contact and thermal sub-problems. The description relies on microstructure based scalar state variables. The formulation follows an approach that considers an instability criterion to define the onset of recrystallization. The analysis is performed for hot forming processes and the kinetics of grain growth is controlled by the grain boundary energies and the energy stored through the dislocation density. A finite element implementation is developed and validated with available numerical and experimental results. In addition, an innovative computational framework is developed for the design of deformation processes using the continuum sensitivity method (CSM) incorporating microstructure related state variables. This CSM involves considering the direct continuum equations, design-differentiating them and then evaluating their discretized form. The developed method is validated by comparing the computed sensitivities to those obtained through a finite difference scheme. In addition, a gradient-based optimization framework is developed which uses the continuum sensitivity method to evaluate the gradients of the objective functions and constraints.

The effectiveness of the method is demonstrated through an example of a two-stage forming process design for producing an axisymmetric disk in 2 stages. The initial billet is a right cylinder of 1.6 mm height and 1.04 mm radius. The height reduction at $r = 0$, in the first stage is 0.3 mm and in the second stage is 0.4 mm. A quarter of the billet is modelled in the simulation and design. The material modelled is taken to be 0.2% C Steel at an initial temperature of 1213 K. The design problem involves a preforming stage using a flat die in an open-die forging process. The finishing stage is a closed die of desired shape. The volume of the billet is chosen so that the final product occupies the finishing die completely. The preforming die surface is represented using a degree 6 Bézier curve with 5 independent variables. The problem is to design the preforming die shape so that the variation in the grain sizes in the finished product is minimized. Figures 8 and 9 present the mean

(a) Initial design iteration



(b) Intermediate design iteration



(c) Optimum design iteration

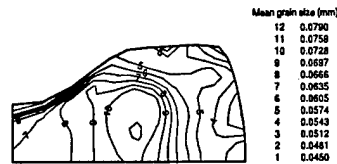


Figure 9: Variation of the mean grain sizes in the final product using various die shapes at different stages of the optimization process.

grain sizes in the intermediate preform (product after stage I) and the finished product. Quantitatively speaking, the average grain size in the product obtained using the guess preforming die shape was observed to be around 64 microns with an average variation of about 40% of the initial grain size. In the product obtained using the optimal die shape, the average grain size was observed to be about 56 microns and the variation was seen to be less than 20% of the initial grain size.

1.5 CSM for the design of deformation processes for polycrystalline materials [8]-[10]

Development of techniques for the control of material properties of polycrystalline materials that are inherently dependent on preferred orientations (texture) is also addressed. To account for the infinite degrees of freedom of microstructural features, a model reduction on the micro-scale was introduced. Reduced-order models are developed to model the evolution of microstructure described by an orientation distribution function using a finite element discretization of the orientation space. This reduced-order modeling approach is based on the technique of proper orthogonal decomposition (POD) and the method of snapshots. Furthermore, novel design problems were introduced and solved for the control of microstructure based on realistic polycrystalline plasticity. Specifically, a gradient based optimization framework is introduced using a multi-length scale continuum sensitivity method (CSM). The model reduction is extended to the sensitivity analysis and is a key element for the success of computational design of deformation processes. In addition, the potential of the presented techniques towards process design for obtaining desired material properties is demonstrated with the control at a material point of the elastic modulus in f.c.c Copper. Here, we control the velocity gradient to obtain a particular distribution of the elastic modulus about the normal direction. The desired distribution is obtained through a uniaxial

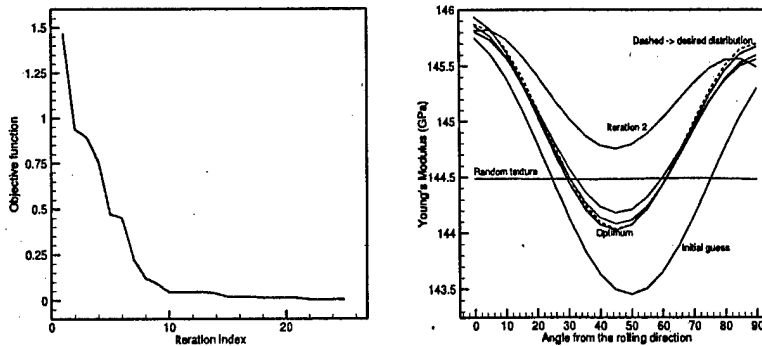


Figure 10: Comparison of the distribution of the elastic modulus at different stages of the optimization process and the variation of the objective function with optimization iterations.

tension test with the velocity gradient expressed in terms of α as:

$$\alpha = \{0.6, 0, 0, 0, 0\}; \quad \alpha_6 = \alpha_7 = \alpha_8 = 0 \quad (1)$$

where α is defined as

$$\begin{aligned} L = & \alpha_1 \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & -0.5 & 0.0 \\ 0.0 & 0.0 & -0.5 \end{bmatrix} + \alpha_2 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & -1.0 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0.0 & 1.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} + \\ & + \alpha_4 \begin{bmatrix} 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} + \alpha_5 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix} + \alpha_6 \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} + \\ & + \alpha_7 \begin{bmatrix} 0.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} + \alpha_8 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -1.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix} \quad (2) \end{aligned}$$

and L is the velocity gradient at a material point and is incompressible. The elastic modulus is evaluated from the polycrystal stiffness (of Copper) where the weighting factor is the ODF expressed over the fundamental region. The initial guess of the velocity gradient was chosen around the design solution as

$$\alpha = \{0.4, 0.1, 0, 0, 0\} \quad (3)$$

Figure 10 compares the distribution of the elastic moduli (about different axis rotated around the RD) at different stages of the design process. Also shown in the Figure 10 is the desired distribution (shown with dashed lines) and the distribution obtained from a random texture (i.e. isotropic material). The optimum velocity gradient was obtained as:

$$\alpha = \{0.674, 0.142, 0.082, -0.012, 0.029\} \quad (4)$$

More examples involving both full and reduced order models are described in [8, 9].

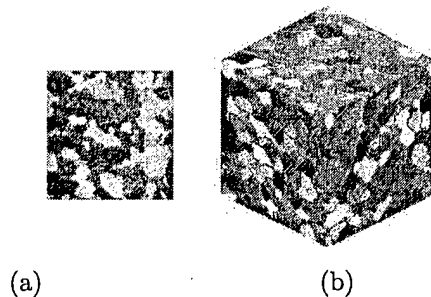


Figure 11: (a) Polarised light micrographs of Aluminum alloy AA3002 representing the rolling plane ($600 \times 600 \mu m^2$). (b) A representative image from the reconstructed class of the image (edge length = $600 \mu m$)

1.6 Classification methodology for microstructure [11]-[12]

A microstructure classification framework has been developed based on support vector machines, an efficient statistical learning technique. Computationally or experimentally obtained microstructure models have been combined with classification and database based approaches for applications of three-dimensional reconstruction and reduced representation of microstructural images. Statistical learning approaches provide an attractive and computationally viable solution to the 3D representation of complex microstructures given limited information over a planar section [11, 12]. The objective of microstructure reconstruction is to mimic the geometry of real microstructure, enabling the creation of numerical realizations that can be applied to the prediction of engineering properties.

The reconstruction has been tested for polyhedral (Figure 11) and two-phase microstructures (Figure 12) and verified with predictions based on stereological analysis and property bound analysis. Since lower order features are employed for classification, the reconstruction eventually yields a class of microstructures instead of a single spatial image. This is because lower-order features used for classification do not uniquely characterize material microstructure, i.e. several different microstructures might have the same lower order functions. Instead of using several higher order measures for the representation of such microstructures, an incremental principal component analysis technique is introduced for reduced representation and quantification. The method (Figure 13) works in conjunction with classification to dynamically update the quantification based on fresh images added to the library and aids in the real-time representation of images [11].

1.7 Materials design through texture data-mining [15]

In [8, 9] we had proposed a multi-scale process design algorithm based on reduced representation of ODF using proper orthogonal decomposition employing the finite element representation of the ODF over an explicit discretization of the orientation space. In a recent work [15], we have further extended the methodology presented in [8, 9] and have

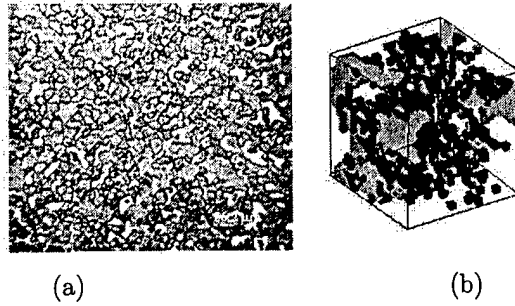


Figure 12: (a) Experimental image of Ag-W composite. (b) A reconstructed pore structure (edge length = $20\mu\text{m}$)

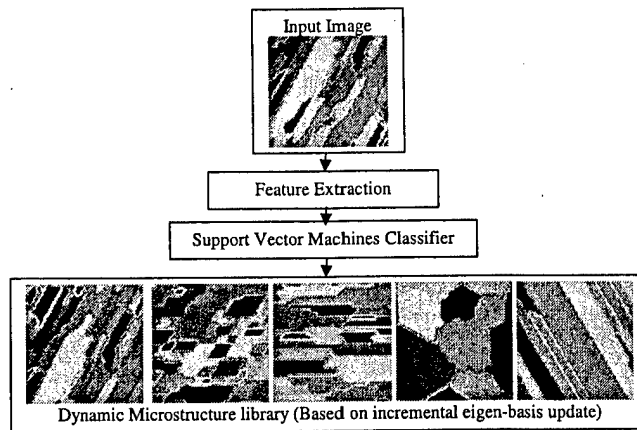
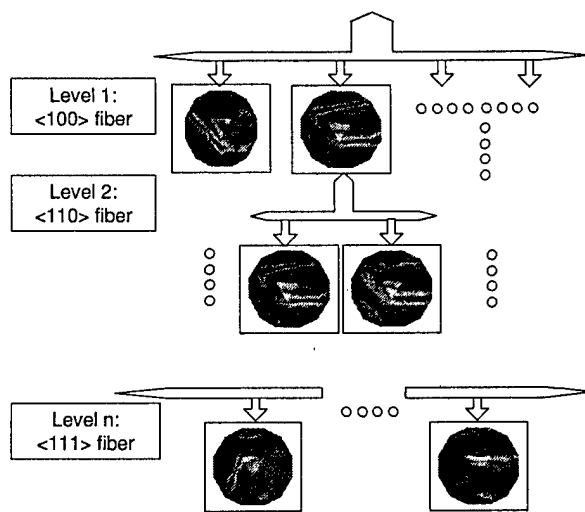
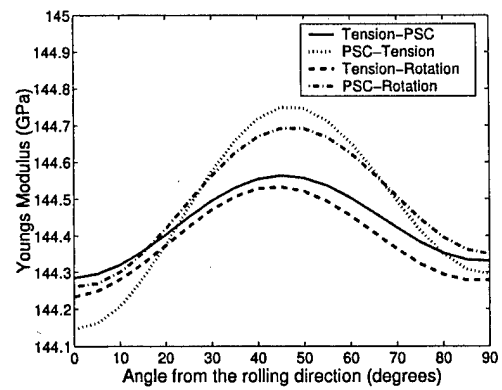


Figure 13: Dynamic library of microstructures based on support vector machine classification and reduced representation using incremental principal component analysis



(a)



(b)

Figure 14: (a) The classification hierarchy for ODFs. The feature vector contains the pole density functions at different sample directions for the family of fibers specified at each classification level. (b) Classification based on property distribution: Young's modulus distribution of a class of ODFs with the process paths indicated. Through data-mining approaches, identification of several processing paths that can lead to a desired texture or texture-dependent property is made possible.

formulated a new data-mining and an adaptive reduced-order optimization approach for the design of appropriate processing sequences that lead to desired properties. ODFs from experiments or direct simulations of texture evolution are stored within a database from which processing routes leading to desired properties can be identified through data-mining. Class hierarchies of ODFs are created based on features in the form of pole density functions over prominent fiber families in the fundamental region (See Fig. 14 (a)). Several processing paths are associated with each class of textures (See Fig. 14 (b)), enabling identification of multiple processing sequences that can lead to the desired properties. Once the processing sequences and associated parameters are identified through classification, fine-tuning of the parameters is performed through an adaptive reduced-order gradient-based optimization approach.

1.8 Development of a 3D design simulator - Transition from academic problems to complex industrial applications

Although simulation of metal forming processes using modern computational tools has reached an advanced stage, there is still a great need to develop computational techniques for process design. In this effort, the continuum sensitivity method (CSM) is extended to three-dimensions (3D) to accurately compute sensitivity fields and drive the design problem with specific material and process objectives. The current 3D developments involve a novel regularized approach to the contact sensitivity problem that addresses the non-differentiability of the contact constraints. The computed sensitivity fields are used in a gradient optimization framework for process design (optimization) in 3D metal forming applications. A typical design problem at each optimization iteration involves simultaneous solution of a direct problem and a number of sensitivity problems corresponding to each of the design variables. Various industrially relevant 3D design problems related to preform and die design for desired properties in the final product are considered in [13, 14] highlighting the features and potential of the present metal forming design simulator.

As an illustration, we highlight the problem (described in [14]), of forging of a circular disc. The objective is to design the preform of variant volume for a final forged product (with fixed stroke) such that the die cavity is fully filled. The workpiece material considered is made of a porous Fe-2%Si with an initial void fraction of 5%. As a result, the volume of the material changes when it is subjected to deformation. In the regions where there are compressive stresses, the void fraction decreases leading to a decrease in volume. The converse happens in regions of tensile stresses. Thus this problem involves not only estimating the optimum preform shape but also the optimum initial volume such that the die cavity is filled. One way to ensure that the die cavity is filled is to consider a preform of a much larger volume than that needed. In this case, the die cavity is filled up but there will be considerable material wastage due to flash.

The design objective in this example is thus posed as computing the optimum preform shape and its volume which fills the die cavity with minimum flash for the given die stroke. The optimization iterations start with a preform of slightly lesser volume than the die cavity and



Figure 15: Initial preform and final forged product for the closed die forging problem.



Figure 16: Optimal preform and final forged product for the closed die forging problem.

the design iterations try to attain the optimum volume and shape of the final preform which fills the die cavity with minimum flash. The initial preform is assumed to be a cylinder of radius 1.0 mm and height 1.44 mm. The preform is subjected to a total deformation of 58% (height reduction from 1.44 mm to 0.6 mm at the center). The workpiece is isothermal with a constant temperature of 1273 K. Using symmetry only one-eighth of the domain is used for computations. A mesh consisting of 600 elements and 819 nodes is used in this simulation. The curved surface parameterization for the preform is performed through a Bézier surface. Figure 15 shows the guess preform and the final forged product for the first optimization iteration. The optimal solution for the design problem is attained in 5 optimization iterations. The optimal preform shape and the final forged product are shown in Figure 16. The volume of the optimum preform is 5.305 mm^3 , and the volume of the final forged product is 5.205 mm^3 . The volume of the die cavity is 5.104 mm^3 .

Several issues remain to be addressed to allow the 3D design simulator to be used routinely in industry. These issues currently being addressed with AFOSR support include algorithms for remeshing and data transfer, implementation of parallel PETSc-based algorithms for increasing the efficiency and performance of the simulator, and other.

1.9 Investigating the role of uncertainty in continuum system analysis and design

Any computational model of complex phenomena that depicts real life behavior has uncertainty built in. The uncertainty may be due to inherent variability of the physical system, approximations in the formulation of the problem, modeling errors in the solution of the approximate model, the lack of information about the system parameters or simply inefficiency in obtaining certain data. Simulation of deformation processes cannot be reliable without quantifying the role that uncertainty plays on model predictions. Uncertainty management

is critical in an accelerated insertion of any process or in product development where engineers need to provide robust design solutions to uncertain requirements with multiple design-related product performance attributes.

With respect to process modeling, we are first interested to quantify how uncertainty in materials and process parameters (model parameters and initial/boundary conditions) propagates in the solution process. Such analysis will allow us to quantify the level of acceptable variability in the material and process data that result in a desired level of robustness of the solution.

With an understanding of the uncertainty propagation in the direct system/process response, we are then interested to address computational design of processes to obtain a product with desired robustness of material properties, geometry and/or microstructure. Robust computational design is addressed with two sub-problems:

- With given product of desired robustness, compute the full statistics of the design variables as well as the acceptable level of uncertainty in the material process data.
- With the computed acceptable level of uncertainty in the material and process data, evaluate the needed material testing that can result in the estimation of this data (materials testing driven by design).

Considering the complexity of addressing uncertainty propagation in deformation processing (which was not the main focus of this project), we explored various uncertainty propagation techniques for 'simpler continuum problems' thus building the needed computational tools to proceed addressing robust design of processes (which is one of the focus areas of our current AFOSR contract). Some of the completed developments in this direction under this grant include the following:

- Development of a MCMC-based Bayesian inference computation framework for estimation of probability distributions of material parameters and as an alternative approach to robust design [16]–[19]
- Investigation of the role of stochastic modeling in multiscale problems: Can a complex system be modeled by representing the dynamics of neglected spatial and time length-scales (subgrid) with stochastic processes? [20]–[22]

Emphasis of our work was given to the development of stochastic modeling, optimization and design tools that can be applied to a variety of systems governed by partial differential equations. For example, considerable effort was applied in identifying efficient algorithms that exploit the inherent structures in the spectral stochastic framework and allow for accelerated probabilistic simulations. Digital libraries that compute statistical averages, efficient finite element assembly algorithms are a part of this venture. Stochastic optimization techniques are also explored for robust design of continuum systems.

We finally at closing note that these developments in investigating the role of uncertainty in continuum systems have indeed been very useful as our first publication on the role of uncertainty in large deformation processes is currently under preparation!! [23].

2 Personnel supported

N. Zabaras (PI), S. Akkaram (GRA, PhD 2001), S. Ganapathysubramanian (GRA, PhD 2004), Swagato Acharjee (GRA), Veeraraghavan Sundararaghavan (GRA), Velamur Asokan Badri Narayanan (GRA, supported in part) & Jingbo Wang (GRA, supported in part).

The PhD theses of Dr. A. Srikanth [24] and Dr. Ganapathysubramanian [25] address many of the developments highlighted in this final report.

3 Interactions with AFRL and industry

- This project was initiated by the Materials Process Design group of AFRL/MLLM. In addition to this division, the Metals Branch of AFRL (Dr. Rollie Dutton) has also been involved in many aspects of this work. The developments related to statistical learning and multiscale modeling and design in materials are direct by-product of our collaboration with them. Many of the accomplishments in this direction are of significance to various DARPA programs including AIM and Prognosis.
- In addition to AFRL/MLLM, companies interacting with us on this project include: General Electric R&D, General Electric Aircraft Engines, Pratt and Whitney (P&W), Alcoa and Mil-Tec corporation.
- Our collaboration with Alcoa has continued towards the experimental evaluation of computational designs, on the designs of flat-die extrusion and multiple-pass rolling processes as well as on the design of processes for damaged materials.
- Plans have been in place with MilTec corporation (<http://www.mil-tec.com>, Dr. Garth Frazier) and AFRL for potential commercialization of the developed simulator. We expect these efforts to materialize in the Spring of 2005.
- The PI has also reviewed this project in various agencies and universities including Alcoa (2001), DARPA (2001), Michigan State University (2002), General Electric R&D (2002), PUCE (Brazil) (2002), GE R&D (2003), COMPLAS 2003 (April 2003), AFOSR (May 2003), AFRL (July 2003), Johns Hopkins University (2003), Worcester Polytechnic Institute (November 2003), Lehigh (January 2004), Duke (February 2004), ARO (April 2004), and AFOSR (May 2004). For more details on these presentations and downloading the actual presentations, see <http://www.mae.cornell.edu/zabaras/>.

Note: The following publications acknowledge the AFOSR support. They are available on line at <http://www.mae.cornell.edu/zabaras/Publications/Publications.html>. Additional powerpoint presentations at conferences, seminars, etc. can also be downloaded from this web site.

References

- [1] N. Zabaras, A. Srikanth, An object-oriented programming approach to the Lagrangian FEM analysis of large inelastic deformations and metal forming processes, *Int. J. Numer. Methods Engrg.* 45 (1999) 399–445.
- [2] A. Srikanth, N. Zabaras, Shape optimization and preform design in metal forming processes, *Comp. Methods Applied Mech. Engrg.* 190 (2000) 1859–1901.
- [3] N. Zabaras, A. Srikanth, Y. Bao, W.G. Frazier, A continuum Lagrangian sensitivity analysis for metal forming processes with application to die design problems, *Int. J. Numer. Methods Engrg.* 48 (2000) 679–720.
- [4] S. Ganapathysubramanian, N. Zabaras, A continuum sensitivity method for finite thermo-inelastic deformations with applications to the design of hot forming processes, *Int. J. Numer. Methods Engrg.* 55 (2002) 1391–1437.
- [5] S. Ganapathysubramanian, N. Zabaras, Computational design of deformation processes for materials with ductile damage, *Comp. Methods Applied Mech. Engrg.* 192 (2003) 147–183.
- [6] N. Zabaras, S. Ganapathysubramanian, Q. Li, A continuum sensitivity method for the design of multi-stage metal forming processes, *Int. J. Mech. Sciences* 45 (2003) 325–358.
- [7] S. Ganapathysubramanian, N. Zabaras, Deformation process design for control of microstructure in the presence of dynamic recrystallization and grain growth mechanisms, *Int. J. Solids Struct.* 41 (2004) 2011–2037.
- [8] S. Acharjee, N. Zabaras, A proper orthogonal decomposition approach to microstructure model reduction in Rodrigues space with applications to the control of material properties, *Acta Materialia* 51 (2003) 5627–5646.
- [9] S. Ganapathysubramanian, N. Zabaras, Design across length scales: A reduced-order model of polycrystal plasticity for the control of microstructure-sensitive material properties, *Comp. Methods Applied Mech. Engrg.*, in press.
- [10] S. Ganapathysubramanian, N. Zabaras, Modeling the thermoelastic-viscoplastic response of polycrystals using a continuum representation over the orientation space, *Int. J. of Plasticity*, in press.

- [11] V. Sundararaghavan and N. Zabaras, A dynamic material library for the representation of single phase polyhedral microstructures, *Acta Materialia*, submitted for publication.
- [12] V. Sundararaghavan and N. Zabaras, Classification of three-dimensional microstructures using support vector machines, *Computational Materials Science*, in press.
- [13] S. Akkaram and N. Zabaras, An updated Lagrangian finite element sensitivity analysis of large deformations using quadrilateral elements, *Int. J. Numer. Methods Engrg.* 52 (2001) 1131–1163.
- [14] Swagato Acharjee and N. Zabaras, The continuum sensitivity method for the computational design of three-dimensional deformation processes, *Comp. Methods Applied Mech. Engrg.*, in press.
- [15] V. Sundararaghavan and N. Zabaras, On the synergy between classification of textures and deformation process sequence selection, *Acta Materialia*, submitted for publication.
- [16] J. Wang and N. Zabaras, A Bayesian inference approach to the stochastic inverse heat conduction problem, *International Journal of Heat and Mass Transfer*, 47 (2004) 3927–3941.
- [17] J. Wang and N. Zabaras, Using Bayesian statistics in the estimation of heat source in radiation, *International Journal of Heat and Mass Transfer*, in press.
- [18] J. Wang and N. Zabaras, Hierarchical Bayesian models for inverse problems in heat conduction, *Inverse Problems*, submitted for publication.
- [19] N. Zabaras, Inverse problems in heat transfer, chapter 17, in the *Handbook of Numerical Heat Transfer*, 2nd Edt., John Wiley & Sons, December 2004 (W.J. Minkowycz, E.M. Sparrow, J. Y. Murthy, eds.)
- [20] V.A. Badri Narayanan and N. Zabaras, Stochastic inverse heat conduction using a spectral approach, *International Journal for Numerical Methods in Engineering*, 60/9 (2004) 1569–1593.
- [21] V.A. Badri Narayanan and N. Zabaras, Variational multiscale stabilized FEM formulations for transport equations: stochastic advection-diffusion and incompressible stochastic Navier-Stokes equations, *Journal of Computational Physics*, in press.
- [22] V. A. Badri Narayanan and N. Zabaras, Using stochastic analysis to capture unstable equilibrium in natural convection, *Journal of Computational Physics*, submitted for publication.
- [23] S. Acharjee and N. Zabaras, Uncertainty propagation in finite deformation plasticity – A spectral stochastic Lagrangian approach, *Computer Methods in Applied Mechanics and Engineering*, in preparation.

- [24] A. Srikanth, A continuum sensitivity analysis of large deformations with applications to metal forming design, Ph.D. Dissertation, Sibley School of Mechanical and Aerospace Engineering, Cornell University, January 2001.
- [25] S.Ganapathysubramanian, Design of deformation processes: Extending phenomenological and polycrystalline plasticity models towards the control of microstructure-sensitive properties, Ph.D. Dissertation, Sibley School of Mechanical and Aerospace Engineering, Cornell University, August 2004.