Final Progress Report

Microstructure Sensitive Design:
A Quantitative Approach to New Materials Development

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Statement of the Problem Studied

Microstructure refers the myriad details of spatial placement of local state (phase, chemistry, lattice orientation, etc.) in heterogeneous materials. It also comprises the defect state, such as dislocation density, vacancy concentration, etc. The relationships between microstructure and effective (macroscopic) properties have been of central focus for the discipline of materials science & engineering for more than a century. Complete, quantitative descriptions of microstructure are enormously complex, and lie well beyond our grasp for most materials of interest. Also, the details they might contain can easily lie beyond the current ability of microstructure-properties relations to absorb them. What is desirable is concurrent development of quantitative representations of microstructure (always requiring these to be experimentally accessible), and associated homogenization methodology, using the available representations of microstructure for estimations of effective properties with sufficient accuracy to be useful to the design application of interest. The foregoing is a robust statement of the central aim of the microstructure-properties leg of the 20th century materials science and engineering paradigm. (Similar statements can be made for the processing-microstructure leg, but these are of less interest to the reported research.)

As we now enter the 21st century it has become apparent, however, that a difficult problem exists in the traditional paradigm of materials science and engineering. The problem lies with the long cycle times required to develop new materials or new microstructures for specified design requirements. Whereas essentially all aspects of multidisciplinary design involving the geometry have been accelerated by the emergence of powerful computers, and suites of software for geometric modeling, finite element analysis, tolerance matching, assembly, and optimization of these, etc., comparable acceleration of changes in materials and materials microstructure have not occurred. It still takes up to a decade to introduce a new material into a complex engineered system, whereas geometrical evolvements may require only days. The consequence of this disparity in design times, between geometry and materials, is an unfortunate marginalization of materials science and engineering as a full contributor to multidisciplinary design.

The research reported here addresses an important component of accelerating materials design. This component can be stated as a problem: even if robust and accurate homogenization relations have been developed, they are often not invertible. In other words, if the desired properties are stipulated as objectives and constraints in a design problem, uni-directional homogenization relations proceed from the microstructure to the properties; and these offer only very limited help to the problem of rapid materials design. It is often prohibitively expensive, in terms of computational resources and in terms of the resources of human imagination, to enumerate or sample even a tiny fraction of all possible material microstructures, and their associated properties. Hence, materials design based upon only forward, uni-directional homogenization relations, is very much limited in promise.

The purpose of the project, entitled *Microstructure Sensitive Design: A Quantitative Approach to New Materials Development*, has been to develop a promising new methodology for microstructure design. Microstructure Sensitive Design (MSD) comprises a highly-invertible approach to the design of microstructure at the mesoscale. This project was funded by the Army Research Office over the period June 1, 2001 – May 31, 2004, and is now continuing with a new grant. The purpose of this report is to briefly describe the most important results and outcomes of the first three years of the project. These have been aggressively reported in 7 journal articles, 12 conference papers (with presentation) and 13 (unpublished) oral presentations.

Summary of the Most Important Results

The central purpose of the investigation has been to develop a fully-invertible methodology for designing mesoscopic aspects of microstructure to meet specified requirements of the designer. The focus has been basic mechanical properties, such as elasticity and initial yield, although the methodology is compatible with any set of properties for which adequate homogenization relations exist. The novelty of the methodology lies in expressing both microstructure and homogenization relations in an appropriate Fourier space. In the Fourier framework a remarkable inversion of the traditional materials science paradigm is achieved, enabling classes of microstructure to be defined for specified sets of required properties: Upon specifying the desired properties and constraints for a particular design problem, recovery of the complete class of microstructures that are predicted to satisfy these requirements is rapidly achieved.

This summary is divided into five parts. Part I describes MSD developed for first-order homogenization relations. These require only the quantitative description of the local state space and its distribution, but nothing of spatial placement of local state enters the picture. Part II describes progress of the work towards introducing MSD as a component of multidisciplinary optimization. Part III describes limited work aimed at deformation processing. In other words, given a class of microstructures that is predicted to meet designer specifications on properties, and given an initial microstructure of the material, can one or more paths of deformation processing be identified that are predicted to achieve the desired class of microstructures. Part IV describes extensions of the MSD methodology to higher-order constitutive relations, and especially to the pair-correlation functions that describe the geometry and morphology of the constituents of microstructure. Extensions of first-order MSD to the higher-order theories of homogenization is a very challenging problem, and have been a focus of the research program. Finally, Part V describes new work on the variance of properties as a function of the size of 'windows' on the microstructure. Variance of properties is now known to depend upon the pair correlation statistics of placement of local state within the window of interest. Work in progress is addressing this important aspect of materials design.

I. First Order MSD

The MSD project began working with first-order homogenization models. These relate elementary volume fractions of components of microstructure to their associated (mechanical) properties. By way of summary, the first-order methodology introduces the concept of a *microstructure hull* in the Fourier space. This hull is a compact and convex region of the space, centered about its origin. It is also convex in all of its subspaces. It describes all possible local state distribution functions of the type that is required by first-order homogenization relationships. When the homogenization relations themselves are formulated in the Fourier framework, it is found that they comprise families of *property hypersurfaces* (sometimes hyperplanes) that intersect the microstructure hull. These divide the hull into two parts – one part that is predicted to achieve a specified property requirement, and another part that is predicted to fail. Intersections of regions bounded by hypersurfaces identify classes of microstructure that are predicted to satisfy multiple property requirements. Consideration of the set of all possible intersections of the property hypersurfaces defines a *properties closure*, which is the theoretical set of all possible properties combinations (as predicted by the selected

homogenization relations). In other words, properties closures are compact regions in the space of combined properties that are predicted to be possible considering all points in the microstructure hull. They are, in fact, approximations to the famous *G-Closure* that was introduced by mathematicians more than two decades ago[1]. The microstructure hull, properties hypersurfaces and the properties closure are the principal constructs of MSD. Implementation in design involves standard methods of linear analysis and gradient based optimization to search the microstructure hull, and its associated properties closures, to find microstructures that are predicted to be ideal for components. Examples of applications studied include compliant beams and small circular holes that give rise to stress concentrations[2]. The following sequence of five figures (I.1-5) illustrates the main constructs of first-order microstructure design as it was applied to the elastic-plastic stress concentration problem.
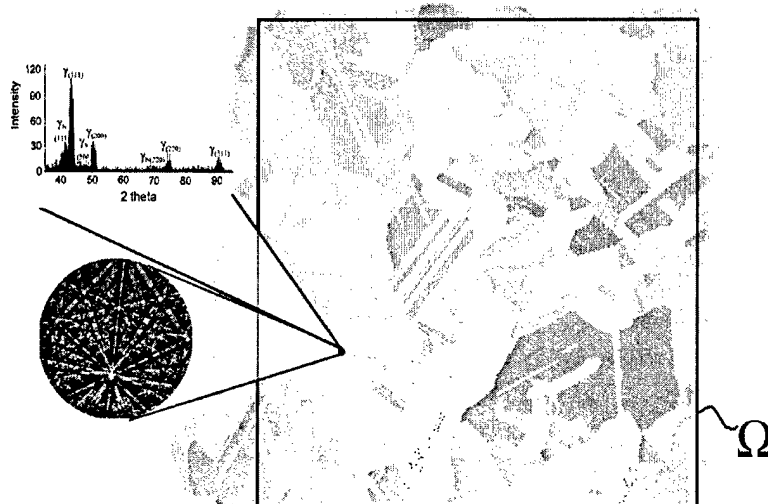

Figure I.1. Illustrating the experimental methods (automated electron backscattered diffraction for crystal phase and lattice orientation, energy dispersive spectroscopy for local chemistry) accessing local state and its distribution in space.

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[1] G-closure refers to the set of all material properties that can be achieved by all possible (spatial) arrangements of a selected set of phases. The notion was introduced by Wiener in 1912, and then formally introduced in connection with problems of G-convergence by Lurie and Cherkaev in 1981. G-closure is known to be an enormously difficult problem, and hence the approximations to G-closure that are obtained by the present body of work are well received.

[2] Recent, continuing work has also considered the crack driving force as an example of the principle of stress concentration in elastic media. Remarkable, order-of-magnitude improvements in crack driving force have been found, but these results are still being scrutinized and independently duplicated before they will be reported.
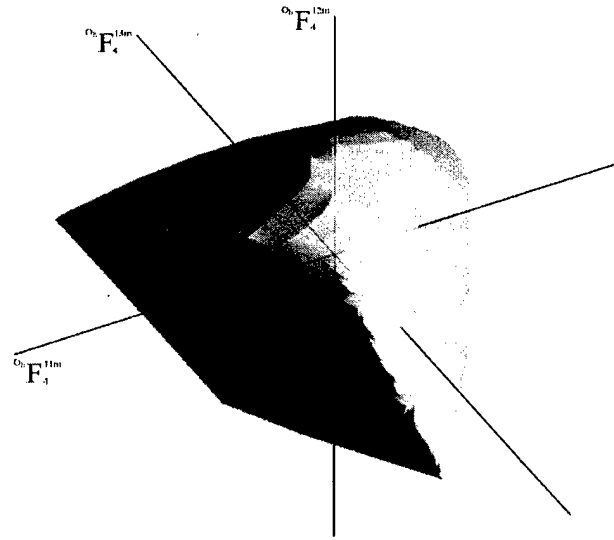
Figure I.2. The 3-dimensional subspace of cubic-orthorhombic texture hull pertinent to the first-order Hill-Paul Bounds. (Lattice orientation is the most complex component of local state space, and crystallographic texture is the central source of anisotropy in mechanical properties.)

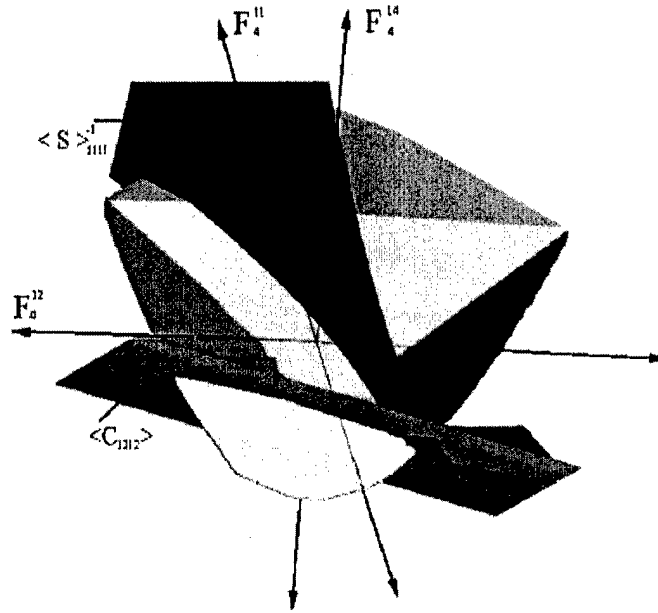Figure I.3. Illustrating specific surfaces for the upper-bound of $C^{eff}_{1212} \leq 63 \; GPa$ (purple plane) and the lower-bound of $C^{eff}_{1111} \geq 330 \; GPa$ for polycrystalline Cu. The yellow region of the texture hull satisfies both bounding relations.
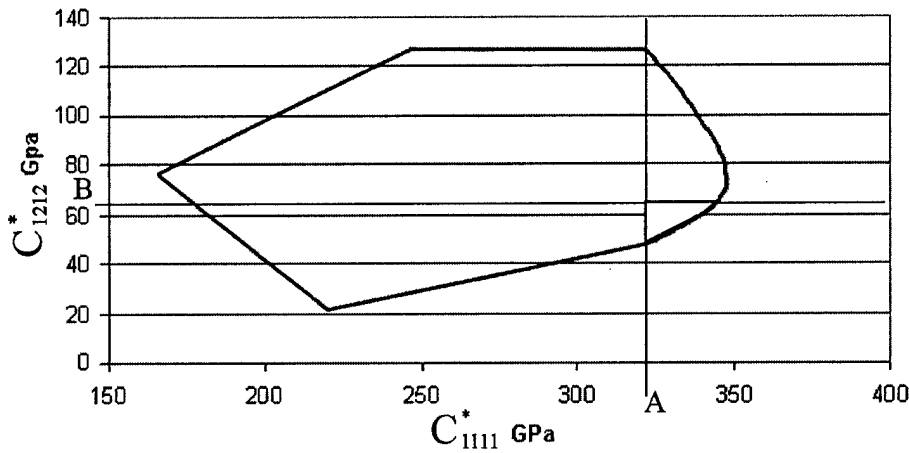
Figure I.4. Properties closure for C_{1212}^{eff} vs C_{1111}^{eff} for polycrystalline Cu, also identifying the combination of properties achieved by the yellow region of the texture hull in Figure I.3.

| Maximum Taylor Factor (Yield Strength) to Stress Concentration (k) Ratio		
Maximum M/K ratio = 1.228		
Taylor Factor = 3.538	Stress Concentration = 2.881	
Texture Coefficients		
$F_4^{11} = -0.462041$	$F_6^{14} = 0.547706$	$F_{10}^{11} = 0.333715$
$F_4^{12} = 0.258893$	$F_8^{11} = 0.167714$	$F_{10}^{12} = -0.27499$
$F_4^{13} = 0.172904$	$F_8^{12} = -0.356061$	$F_{10}^{13} = -0.138081$
$F_6^{11} = -0.485852$	$F_8^{13} = -0.211022$	$F_{10}^{14} = 0.283281$
$F_6^{12} = -0.123046$	$F_8^{14} = -0.605061$	$F_{10}^{15} = 0.176355$
$F_6^{13} = -0.221207$	$F_8^{15} = 0.041599$	$F_{10}^{16} = 0.186187$
$J = 1.830$		
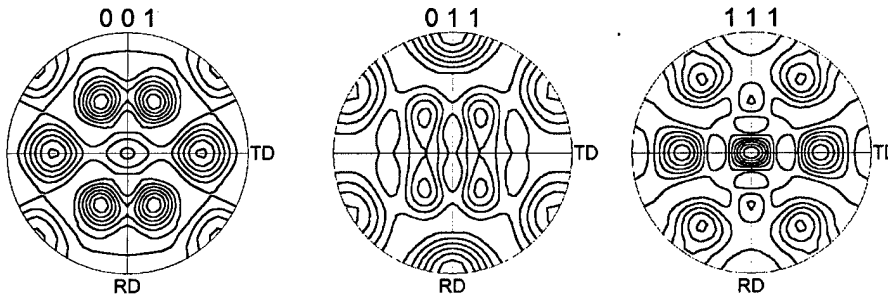
Figure I.5. Fourier coefficients (18) and pole figures obtained for textured Cu polycrystal optimized for load bearing capacity, without yielding in the presence of a circular hole. Performance over all possible textures is predicted to vary by a factor of two.

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II. MSD as a Component of Multidisciplinary Optimization

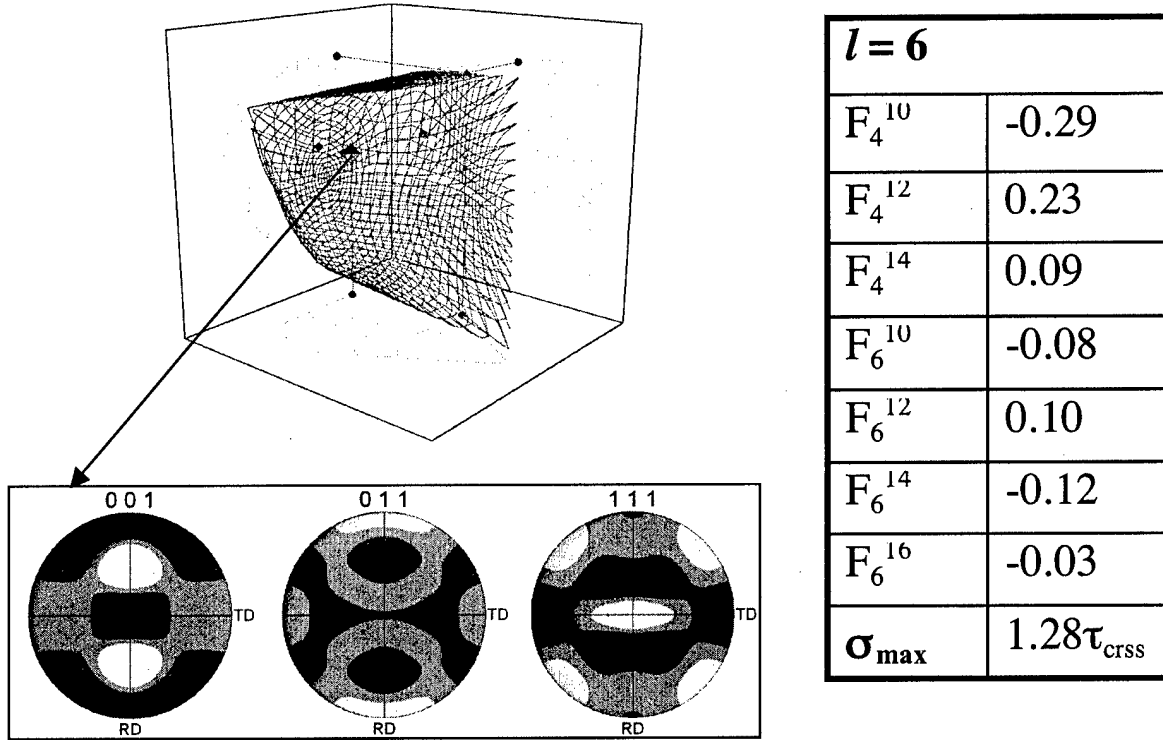| $l = 6$	
F_4^{10}	-0.29
F_4^{12}	0.23
F_4^{14}	0.09
F_6^{10}	-0.08
F_6^{12}	0.10
F_6^{14}	-0.12
F_6^{16}	-0.03
σ_{max}	$1.28\tau_{crss}$

Figure II.1 MSD-FE solution for the design of a thin plate of polycrystalline Nickel with a central circular hole subjected to in-plane tensile load.

In an effort to facilitate MSD as a component of multidisciplinary optimization, we have successfully interfaced the mathematical framework of Microstructure Sensitive Design (MSD) with the finite element (FE) codes typically used by the designer. We have thus far focused on case studies involving elastic-plastic design of mechanical components. However the framework is general enough to be applicable to other multidisciplinary design problems.

More specifically, a design and optimization environment was created using ABAQUS and ANSYS (a finite element codes used extensively in mechanical design) and iSIGHT (an optimization environment used extensively by the design community). As an initial case study, the performance of an orthotropic thin plate containing a circular hole subjected to an in-plane tensile load was considered. For this case an analytical solution is known – as reported in the previous section. The primary design objective was to maximize the load carrying capacity of the plate while avoiding plastic deformation in the plate. If the material is assumed to exhibit isotropic properties, optimizing the performance is trivial; the strongest material will provide the highest load carrying capacity. However, the consideration of elastic and plastic anisotropy induced in the sample during processing operations greatly enriches the design space. Crystallographic texture was assumed to be the main contributor to the anisotropic mechanical properties exhibited by the material. Further, the focus was restricted to polycrystalline nickel. A

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finite element model was created for the thin-orthotropic plate with a central circular hole. Appropriate boundary conditions were applied to simulate in-plane tensile loading of the plate. The Fourier coefficients of the ODF were considered as the design variables. The design and optimization started with a selection of Fourier coefficients inside the microstructure hull. Macroscale properties were estimated using upper bound theories and the performance of the plate was evaluated using ABAQUS. The load at initiation of plastic yield near the hole was evaluated. iSIGHT was used to search through the microstructure hull to arrive at the set of Fourier coefficients that were predicted to correspond to the highest load carrying capacity for the plate. The methods described here indicate that the maximum value the far-field applied stress for this design example can reach is $1.28\tau_{CRSS}$, where τ_{CRSS} denotes the critical resolved shear stress for the material (at the single crystal level). This result represents an improvement of over 200% compared the lowest possible performance for the same design problem. The MSD solutions were validated by direct comparison with finite element simulations that employed a Taylor-type polycrystal constitutive model at each integration point. A good agreement was obtained between MSD predictions and finite element simulations.

A second design study, focused on turbine disks (or 'blisks') has recently been completed at BYU using the ANSYS + iSIGHT software. The elastic calculations focused on elastic crack driving force. The startling result has been an improvement of over one order of magnitude in this driving force. Work is currently underway to check these results, and full reporting will be undertaken later.

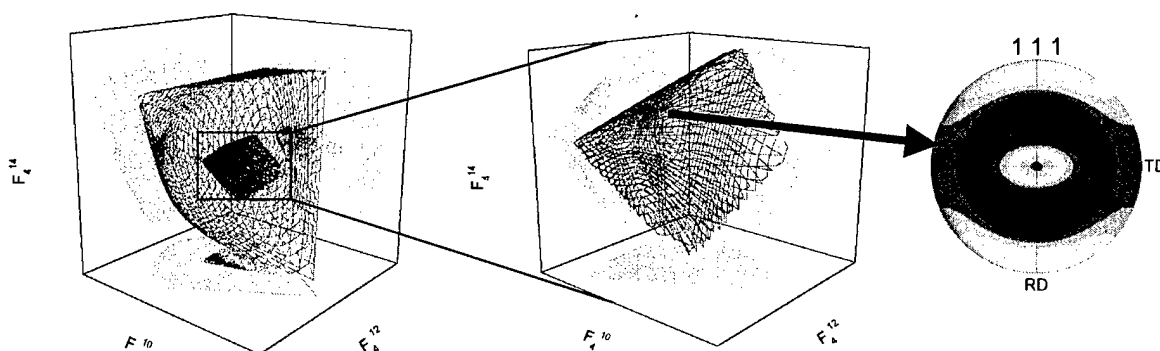### III. Deformation Processing in MSD

Figure III.1. The red wire-framed convex hull denotes the set of all possible textures, while the blue subspace denotes the set of textures that can be produced by a combination of selected processing routes starting with a random initial texture. The pole figure shown is predicted to yield the best performance for the case study described in Section II, when the texture is constrained to lie within the subset of textures that can be produced using selected set of deformation processing operations.

Once a class of desired microstructures is identified, the next step is to find a processing path to physically realize one of the elements of the desired class of microstructures. For the case study mentioned in part II, an optimum texture was identified using the MSD-FE framework. Building on a concept that was originally proposed by Bunge and Esling (1984) for capturing efficiently the details of the evolution of deformation textures in polycrystalline metals, process design solutions were explored. The processing routes considered included only those room

temperature deformation processes that preserved the orthorhombic sample symmetry. Figure III.1 delineates the region corresponding to all physically realizable textures, in the first three component subspace of the Fourier space, as a red wire-framed convex hull. However, not all textures in this convex hull can be realized by the selected set of processing paths; the set of textures that can be produced starting with an initial random texture is depicted as a blue wire-framed region in Figure III.1. The mathematical tools developed allow us to identify the complete set of textures that can be produced, starting from a given initial texture, by an arbitrary combination of selected processing techniques. It is further possible to design a processing route for any selected target texture that lies in this subset of realizable textures (the blue wire-framed subspace in this case study). The ability to address processing solutions in the MSD framework further strengthens and enhances the linkage between designers and materials experts in the engineering design enterprise.

IV. Extension of MSD to Second-Order Homogenization Theory

Within the context of statistical continuum theory, refined bounds and estimates of effective properties require information about microstructure beyond the volume fractions required by the first-order theories. For example, expressions for the fourth-order effective elasticity tensor, C^{eff}, can be expressed as a geometric series in the correlation functions of local stiffness:

$$C^{eff} = \langle C \rangle - \langle C'\Gamma C' \rangle + \langle C'\Gamma C'\Gamma C' \rangle - \dots .$$

Here the angular brackets, $\langle \; \cdot \; \rangle$, denote ensemble averages, $C' = C - C^r$ is the polarization of local stiffness C with respect to a selected reference stiffness, C^r, and Γ denotes an appropriate Green's function operator associated with solutions to the basic governing equations for static linear elastic properties subject to homogeneous boundary conditions. The basic feature of this equation is a hierarchical dependence upon an ascending order of correlation functions; thus, the first-order term requires $\langle C(x) \rangle$, the second-order term $\langle C'(x)C'(x') \rangle$, and so forth. This hierarchy is found in other theories, such as the solution to the Navier-Stokes relations for the viscoplastic modulus.

It is known that homogenization relations based only upon volume-fraction information may be less than adequate to conduct useful design. Elastic bound estimates for polycrystals, for example, are often separated by ~ 10% or more of the estimate itself, and this may be unacceptable in highly-constrained design. It is also known that relations for texture evolution, containing second-order terms in the viscoplastic modulus, correctly predict effects observed in experimental measurements, but not explained by the first-order theory. Thus, there is ample incentive to extend MSD to consider second- and higher-order elements of the homogenization relations. However, the question becomes to what extent the remarkable quality of invertibility, attained in the first-order theory, can be preserved in these extensions.

Invertibility in advanced homogenization relations and their concomitant microstructure representations has been explored (and is continuing to be explored) as an important part of this research project. We have thus far addressed mainly the problem of constructing the hull for 2-point orientation correlation functions, as required, for example, by the second term in the homogenization relation given by relation above. Higher-order homogenization relations become

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accessible if we are able to construct an appropriate hull for the 2-point (pair)correlation functions. This possibility was mentioned early in the earliest work describing the new methodology, but early in the project the complexities of the 2-point representations were not fully appreciated.

The principal challenge associated with the pair correlation functions is a complex interdependency in the r- variable of the representation itself. Consider the joint probability density that the tail and head of a vector, r, randomly placed in the microstructure of a single phase polycrystal, associates with lattice orientations g and g', respectively. In statistically-homogeneous microstructures, this probability density is labeled $f_2(g,g'|r)$; it is also called the *2-point orientation correlation function*, or the *orientation correlation function* (OCF). Modern methods of automated electron backscattering diffraction enable statistically reliable estimates of this function to be obtained by experimental sampling of the microstructure as is illustrated in Figure 1. A limited understanding of the r- interdependence of the OCF can be seen in the following conservation relationship that was derived in this research for statistically homogeneous microstructures:

$$\iiint_{\Psi(\Omega)} f_2(g,g'|r)\theta(r)dr = f(g)f(g').$$

Here, $\Psi(\Omega)$ designates the complete set of all possible vectors r that can be found in any particular region of 3-D space, Ω. When pairs of points are introduced into random and independent locations within Ω, $\theta(r)$ is the geometrical probability density for the occurrence of vector r among these pairs. It is evident that this relation defines a necessary system of constraints, linking the OCFs to one-another. However, the question that arises is whether these constraints are sufficient to insure that a set of OCFs is physically-realizable in the ensemble. Torquato (in his book *Random Heterogeneous Materials*, Springer, 2002) reviewed what is known about the related problem of *physical realizability* for the auto-covariance function in 2-phase composites, and concluded that the problem remains an open and unsolved one. Addressing the r-interdependence of the OCF is the chief obstacle to a formulation of microstructure design at the second-order level.

During the course of this project we explored a number of possibilities for overcoming the r-inter-dependence problem in pair correlation functions. After many failed attempts, a particular approach was developed which is tractable. It is shown that the correlation functions can be expressed in terms of an intermediate construct, called the texture function; the OCFs themselves are shown to have quadratic dependence in the texture functions. A complete (finite) texture hull is readily constructed for the texture functions in Fourier space, and is found to be a convex polytope. Eigen-texture functions occupy the corner (extreme) points of the polytope. Second-order MSD has been shown to then proceed directly (and beautifully) from homogenization relations evaluated at the eigen texture functions (corner points), and weighted as convex combinations according to their occurrence in the ensemble of microstructures. These constructs gives rise to second-order (combined) properties closures, from which refined MSD can proceed.

This new methodology for second-order MSD has only been achieved in our research very recently. The seminal paper on the method has been submitted for publication to Acta Materialia, and is currently in review. Work on representing the spatial placement using Haar wavelet functions has also shown great promise of more efficient representation of optimal eigen-texture functions as compared with other Fourier bases. Here we illustrate the results of a simple case study, based upon the texture obtained by first-order MSD for the load bearing

capacity of Cu plate containing a circular hole, and loaded in tension. Having constrained the texture via first-order MSD, the elastic bounds (first-order, Hill-Paul) are fixed. The question addressed in this case study by second-order MSD is that of optimal placement of components of the texture (i.e., morphological texture) to realize the boundaries defined by the Hill-Paul bounds. A very modest cubical model, consisting of 4x4x4=64 cells was used. Three single crystal components (and their orthorhombic variants) were used to model the optimized plate texture. The results of this limited study are illustrated in Figures IV.1-2.
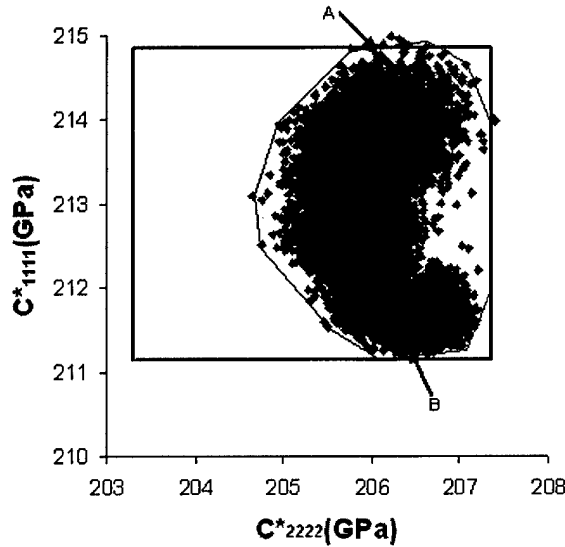

Figure IV.1 Sampling of the C_{2222}^{eff} vs C_{1111}^{eff} elastic properties closure for the Cu polycrystal defined by first-order MSD for the hole-in-the-plate problem (see Figure I.5). 3×10^6 eigen-texture functions were constructed and evaluated to obtain the convex approximation to the second-order closure (surrounded by thin lines). Minor breaching of the Hill-Paul bounds is anticipated when the homogenization relations are truncated at the second-order term.
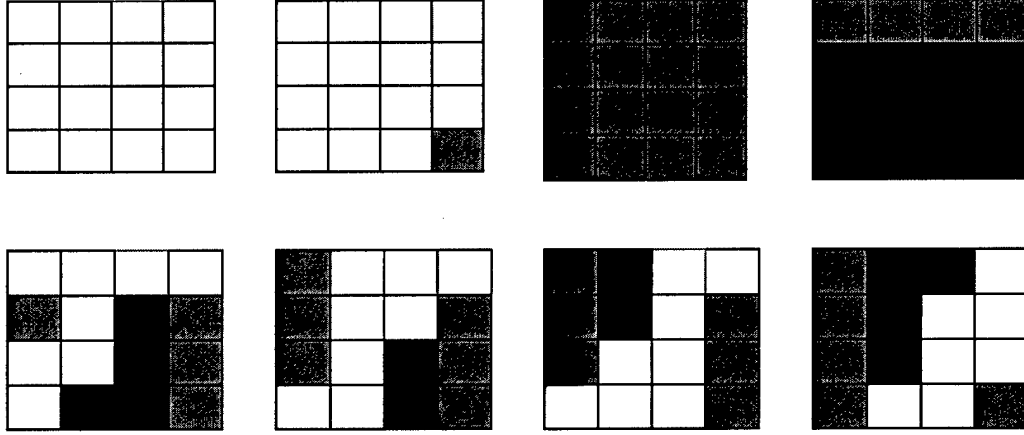
Figure IV.2. Morphology of configurations that maximize C^{eff}_{1111} (point A in Figure IV.1), top row left to right; and minimize C^{eff}_{1111} (point B in Figure IV.1), bottom row left to right. (White boxes contain crystallites of highest C_{1111}, gray are intermediate, and black are lowest.)

V. Treatment of Variance in MSD

It has been known since the work of Lu and Torquato [*J. Chem. Phys.* **93** (1990) 3452] that fluctuations in the local state distribution function in finite volumes of material are closely related to the details of the 2-point correlation functions, or OCFs, over distances spanned by the specified volumes. The original application of this work was in treatment of granularity of photographic media, which is modeled as a 2-phase problem. We have recently extended these original ideas to consider the variance of properties estimated (or bounded) by elementary arithmetic averages. We have obtained the following result for the variance $\sigma^2_{p(\Omega)}$ of property $p(\Omega)$ in statistically placed regions Ω of the 3-dimensional real space:

$$\sigma^2_{p(\Omega)} = \frac{1}{v(\Omega)^2} \iiint_H \iiint_{H'} \iiint_{\Re^3} \left[f_2(h,h'\,|\,\vec{r})p(h)p(h')\Theta(\vec{r}\,|\,\Omega)d\vec{r}dhdh' \right] - \bar{p}(\Omega)^2.$$

Here $v(\Omega)$ is the volume of Ω, $f_2(h,h'\,|\,\vec{r})$ is the 2-point correlation function for probability of occurrence of local state h at the tail and local state h' at the head of sampling vector $\vec{r}$. $p(h)$ is the local property associated with local state h. The function $\Theta(\vec{r}\,|\,\Omega)$ is equal to the volume of intersection of two 3-dimentional regions of identical size and shape, Ω, but whose centers of mass are separated by vector $\vec{r}$. The right-most term is defined by

$$\overline{p}(\Omega)^2 = \left[\iiint\limits_H f(h)p(h)dh \right]^2$$

where $f(h)$ is the local state distribution function and H is the local state space.

Initial application of the foregoing was to estimate the variance of the R-parameter (ratio of width to thickness strains in tensile deformation) using an elementary plasticity model (Sachs quasi-lower-bound model). The results were encouraging, and several aspects of the variance equation were tested. At the present time the work is being extended to a Taylor yielding model, which is more broadly accepted in crystal plasticity. An experimental program based upon tensile testing and stretch forming of HSLA steels at various ratios of grain size/thickness is being pursued. The initial results of this component of the project were presented at Numiform 2004, and included as a paper in the published proceedings.

Publications and Technical Reports

Papers published in peer-reviewed journals

M. Lyon and B. L. Adams, *Gradient –Based Non-Linear Microstructure Design* J. Mechanics and Physics of Solids 52 (2004) 2569-86.

S. R. Kalidindi, J. Houskamp, M. Lyons, and B. L. Adams, *Microstructure Sensitive Design of an Orthotropic Plate Subjected to Tensile Load,* Int. Journal of Plasticity 20 (2004) 1561-1575.

B. L. Adams, M. Lyon and B. Henrie, *Microstructures by Design: Linear Problems in Elastic-Plastic Design* Int. Journal of Plasticity 20 (2004) 1577-1602.

B. L. Adams and X. Gao, *2-Point Microstructure Archetypes for Improved Elastic Properties* Journal of Computer-Aided Materials Design (2004) in press.

D. S. Li, H. Garmestani and B. L. Adams, *A Processing Path Model for Texture Evolution in Cubic-Orthorhombic Polycrystalline System,* International Journal of Plasticity (2004) in press.

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B. L. Adams, X. Gao and S.R. Kalidindi, Finite Approximations to the Second-Order Properties Closure in Single-Phase Polycrystals, Acta Materialia (2004) submitted.

G. Proust and S. R. Kalidindi, Delineation of elastic and plastic yield property closures for face-centered cubic polycrystals using first order homogenization theories, Journal of Mechanics and Physics of Solids (2005) submitted.

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B. L. Adams, M. Lyon, B. Henrie and S. Kalidindi, *Microstructure by Design,* in Plasticity, Damage and Fracture at Macro, Micro and Nano Scales, eds. A. S. Khan and O. Lopez-Pamies, Neat Press, MD, 2002, pp. 3-5.

M. Lyon, B. L. Adams and B. Henrie, *Microstructure design of compliant beams* in Plasticity, Damage and Fracture at Macro, Micro and Nano Scales, eds. A. S. Khan and O. Lopez-Pamies, Neat Press, MD, 2002, pp. 33-35.

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H. K. Duvvuru and S. R. Kalidindi, *Processing Solutions for Targeted Textures Using Spectral Methods,* DETC2004-57752, Proceedings of DETC2004: ASME 2004 International Design Engineering Technical Conferences And The Computers And Information In Engineering Conference, Salt Lake City, UT, 2004.

S. R. Kalidindi, J. Houskamp and G. Proust, *Coupling of Microstructure Sensitive Design With Finite Element Codes: Design of an Orthotropic Plate With a Circular Hole Loaded in Tension,* DETC2004-57635, <u>invited</u>, Proceedings of DETC2004: ASME 2004 International Design Engineering Technical Conferences And The Computers And Information In Engineering Conference, Salt Lake City, UT, 2004.

S. R. Kalidindi, J. Houskamp, G. Proust, and H. Duvvuru, *Microstructure Sensitive Design with First Order Homogenization Theories and Finite Element Codes,* <u>invited keynote lecture</u>, ICOTOM, proceedings to be published in Materials Science Forum, 2005.

Papers presented at meetings, but not published

B. Henrie , B. L. Adams, S. R. Kalidindi, H. Garmestani, *Microstructure Design by the Spectral Method,* presented at the United Engineering Foundation Conference on Materials by Design, Lake Arrowhead, CA, November 12-14, 2001

S. R. Kalidindi, J. Houskamp, G. Proust, B. L. Adams, and H. Garmestani, *Design of an Anisotropic Plate with a Hole Using Spectral Methods,* 9th AIAA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, Atlanta, September, 2002.

M. Lyon, B. L. Adams and B. Henrie, *Applications of Microstructure Sensitive Design* (MSD), U.S. National Congress on Theoretical and Applied Mechanics, Blacksburg, VA, June 24-28, 2002.

S. R. Kalidindi, B. Adams, and H. Garmestani, *"Microstructure Design and Optimization using Spectral Representations: Novel Tools for the Materials Engineer"*, MRS Spring Meeting, San Francisco, California, April 2002.

J. Houskamp, S. R. Kalidindi, B. Adams, and H. Garmestani, *"Process Design to Achieve Targeted Microstructures: The Spectral Method"*, TMS Annual Meeting, Seattle, February 2002.

S. R. Kalidindi, "Microstructure Sensitive Design: A Spectral Approach to Materials By Design", SES Annual Meeting, Ann Arbor 2003.

J. Houskamp, S. R. Kalidindi *"Robust Materials Design Using Microstructure Sensitive Design"*, Plasticity 2003, Quebec City, Canada, July 2003.

G. Proust and S. R. Kalidindi, "Microstructure Sensitive Design: Elastic-Plastic Property Closures", Plasticity 2003, Quebec City, Canada, July 2003.

B. L. Adams and S. D. Sintay, *Recent Developments in Non-Linear Microstructure Sensitive Design,* invited, Air Force Office of Scientific Research MEANS Workshop, Boulder, CO. August 6-8, 2003.

B. L. Adams, *Microstructure-Sensitive Design: Towards a Fully Invertible Theory of Microstructure Design,* invited keynote address, Army Research Office/Georgia Institute of Technology Workshop on Materials Design, April 2004.

B. L. Adams, *Advances in the Spectral Method of Microstructure-Sensitive Design,* International Conference on Heterogeneous Materials Mechanics, invited keynote address, Chongqing, China, June 2004.

S. Sintay and B. L. Adams, *Object Oriented CAE Software for the Exploration and Design of Microstructures,* Symposium on Materials Design and Optimization, ASME Design Engineering Technical Conference, Salt Lake City, September 2004.

G. Proust and S. R. Kalidindi, *Delineation of the property closures for polycrystalline fcc materials*, TMS Annual Meeting, New Orleans, September 2004.

Educational Workshop

A one-week educational workshop on *Microstructure Sensitive Design* was conducted by the investigators in December 2002 at Drexel University. The workshop was sponsored by Air Force Office of Scientific Research. The primary objective of this workshop was to bring together and expose a highly qualified but diverse group of individuals to the important field of Materials Design Science and Engineering. An exemplary group of experts was assembled to carry out the

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proposed educational activity. The selected individuals brought together internationally recognized expertise in all fields related to MSD. A multi-disciplinary curriculum with the necessary lecture notes and handouts was developed for the workshop. As a follow up to this educational activity, Professors Adams and Kalidindi are now engaged in writing a graduate level textbook on Microstructure Sensitive Design.

Technical reports submitted to ARO

ARO Interim Report #1, June 1, 2001 – December 31, 2001

ARO Interim Report #2, January 1, 2002 – December 31, 2002

ARO Interim Report #3, January 1, 2003 – December 31, 2003

ARO Final Report, this report

List of participating scientific personnel

Brent L. Adams, Professor of Mechanical Engineering, Brigham Young University (recipient of Dusenberry Professorship at BYU in 2002; Keynote address at Georgia Tech/ARO Workshop on Materials Design, April 2004; named Fellow of ASM International in 2004)

Surya R. Kalidindi, Professor and Head of Materials Engineering, Drexel University (scheduled to give plenary address at ICOTOM 14 in Leuven, Belgium, summer 2005, on materials design)

Benjamin Henrie, MS thesis student at Brigham Young University (completed MS with thesis in summer 2002; member of technical staff at Los Alamos National Laboratory)

Josh Houskamp, Ph. D. thesis student at Drexel University (anticipated completion of doctorate at Drexel U in August 2005)

Carl Gao, Ph. D. thesis student at Brigham Young University (anticipated completion of doctorate at BYU in August 2005)

Mark Lyon, undergraduate and graduate student, Brigham Young University (honors thesis, May 2002, recipient of MRS Scholarship, 2001; recipient of NSF Graduate Fellowship, 2002; completed MS thesis in summer 2003; currently pursuing doctorate in applied mathematics at California Institute of Technology)

Steve Sintay, graduate student Brigham Young University, completed MS thesis in December 2004 (currently pursuing doctorate in materials science at CMU)

Craig Przybyla, MS student at Brigham Young University (anticipated completion of MS thesis, August 2005).

Gwenaelle Proust, PhD student at Drexel University (Third place for best student paper in the 2003 SES Annual Meeting, Ann Arbor, Michigan; Zontia International Amelia Earhart Fellowship 2004-2005; anticipated completion of PhD thesis, March 2005; scheduled to start a post-doctoral position at Los Alamos National Laboratory in April 2005).

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13. ABSTRACT (Maximum 200 words)

The central goal of the project is to develop a new spectral method for design of polycrystalline materials. The methodology (MSD) differs from other materials design approaches in that all components of the materials design enterprise are communicated in the same mathematical framework – a Fourier space in which the objectives/constraints of the mechanical designer, the set of all possible material microstructures, and the set of all possible combined properties are examined in a common framework. During the three year period of the project we have tackled the challenging problem of fully developing the first-order MSD and then extending it to its second-order framework, by incorporating 2-point correlation functions in the homogenization relations. We have also conducted the first numerical tests of method for evolving 1-point microstructure statistics during plastic deformation. The main achievements include (1) new methodology for estimating properties closures via MSD, (2) a framework in which 2-point homogenization can be addressed by MSD, (3) an interface between MSD and multidisciplinary optimization, and (4) demonstration of benefits to be achieved in selected design projects, especially including geometries that concentrate stress.

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