THE CHALLENGE FOR MATERIALS DESIGN

Integrating Modeling and Computation

presented at

NATO Advanced Research Workshop

Metallic Materials with High Structural Efficiency

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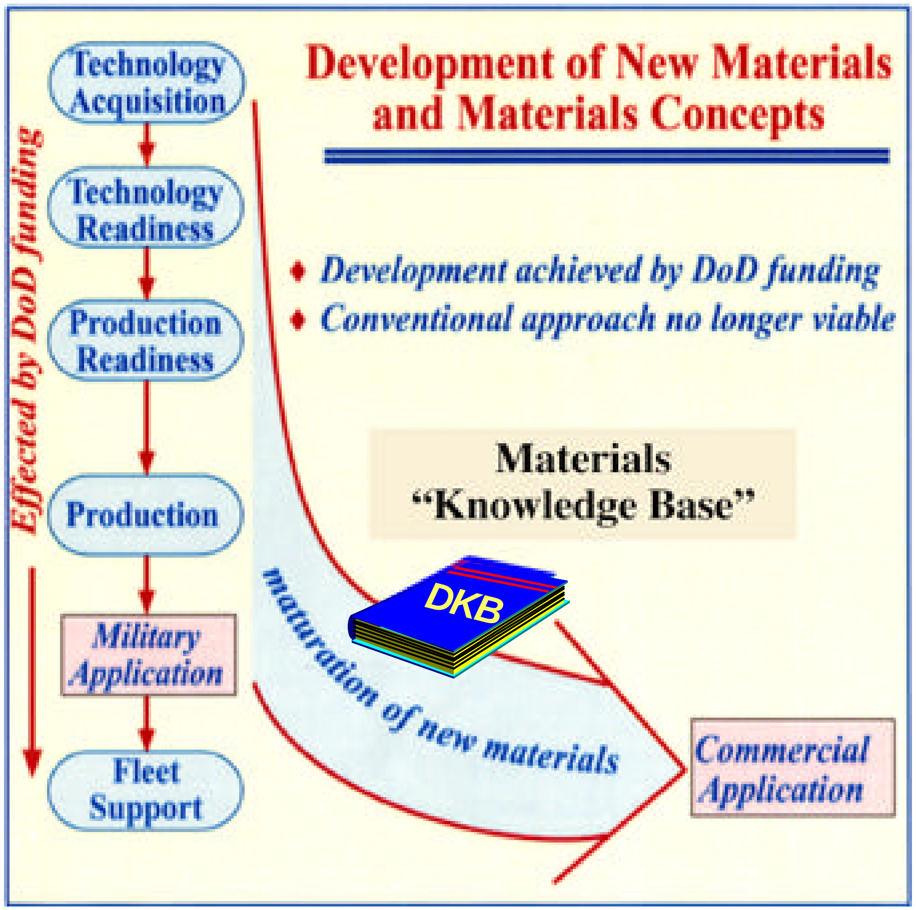
Outline

- Introduction
- MEANS
  - Philosophy of the Program
  - Projects in Structural Metallic Materials
- Critical Areas for Future Research
  - Physics-based Model Development and Verification
  - The Quantitative Description of Structure
  - Experimental Techniques
  - The Designer Knowledge Base
  - Integration of Materials Models with Engineering Design
- Conclusions

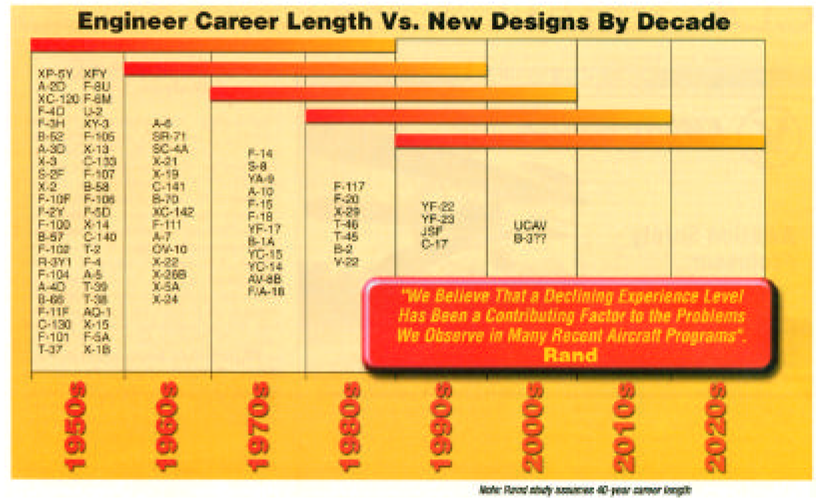
The Issue

- Materials Science and Engineering has not progressed as rapidly as other disciplines in contributing to the reduction in the product cycle during the last decade.
- New developments in materials are not being exploited as rapidly as desirable because of the time and cost necessary to obtain information on material properties and characteristics.
- Products are being designed and fabricated with existing materials having verified design properties, resulting in the use of less than optimal materials for many applications.

Aerospace Structural Materials Development: How It Happened



Adapted from Fraser, 1998; Wax, 1999



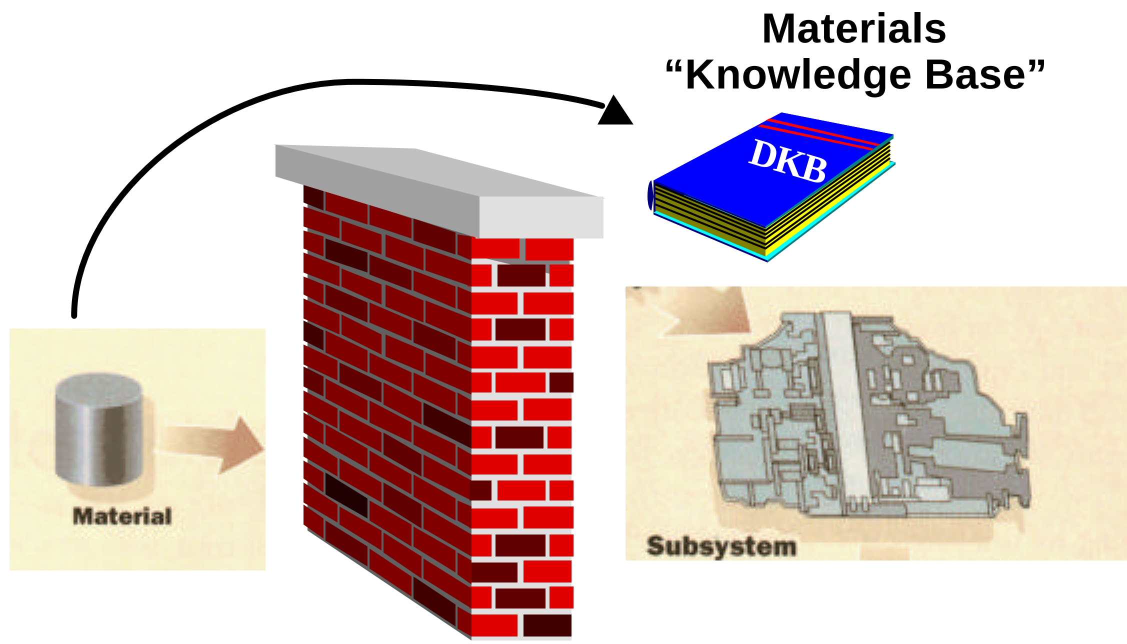
- DoD materials transition opportunities (systems) have drastically reduced
- Material development time far exceeds the modern short product cycle
  - iterative, empirical development of "Knowledge Base" is lengthy, data intensive, and expensive

21st Century Reality Demands that the Paradigm Change!

The Disconnect!

Major disconnect between materials development & components/systems engineering design

- Known alloy to reliable part ~36 months
- Steels for navy landing gear 15+ yrs
- Lightweight composites for army vehicles 15+ yrs
- Gamma titanium aluminides ~30yrs and counting
- Ceramics for engines - 30+++ ? yrs
- Evolutionary alloy changes (ship steels, superalloys, etc) ~7-10 years



Materials Development

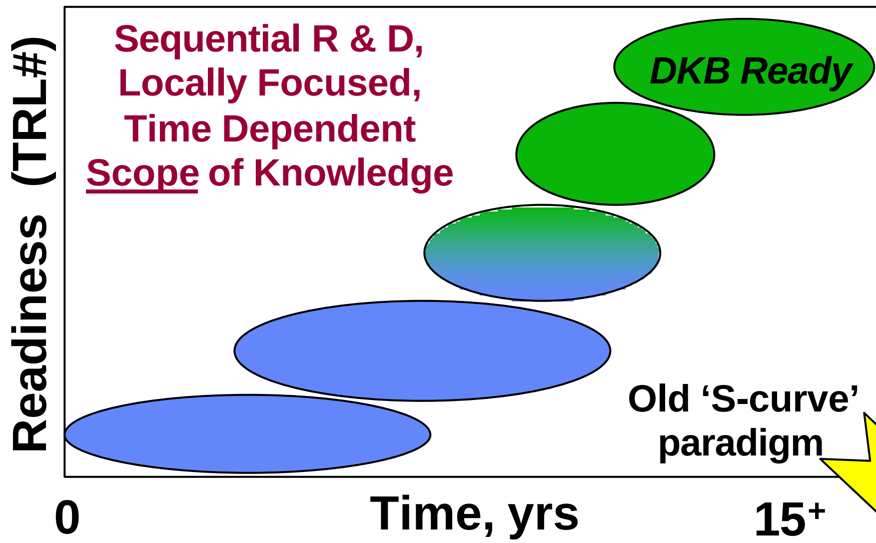
- Highly Empirical
- Testing Independent of Use
- Existing Models Unlinked

Engineering Design

- Materials Input from "Knowledge Base" of Data (Data Sheets, Graphs, Heuristics, Experience, etc.)
- System/Sub-System Design is Heavily Computational and Rapid
- Well Established Testing Protocols

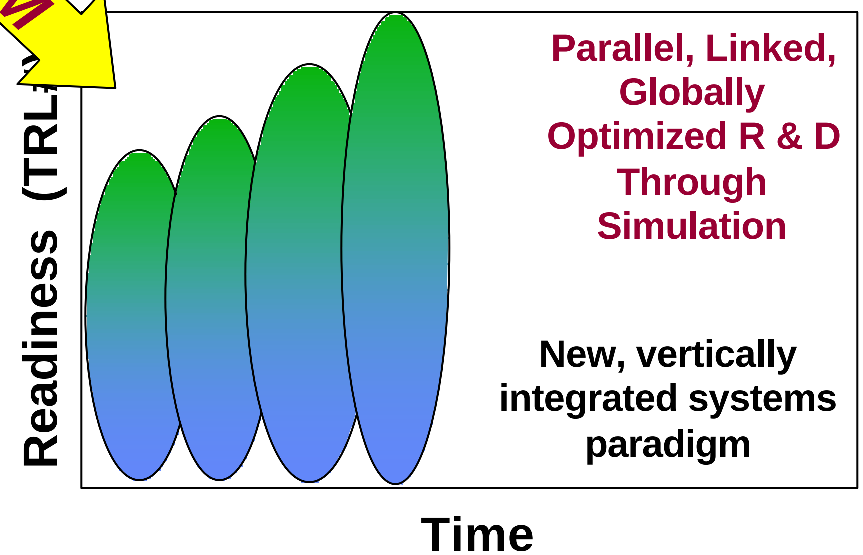
Adapted from Wax, 1999

AIM Paradigm for Materials R & D



- Sequential M & P
- Optimized from heuristics
- "Designer Knowledge Base" NOT Ready Until Final Stages

- Building "Designer Knowledge Base" begins at outset
- Optimization based on <u>design IPT need</u>
- Time & effort refines <u>quality</u> of knowledge base, <u>not its scope</u>



Adapted from Wax, 1999

Materials Engineering for Affordable New Systems

Exploit computational Materials Science and Engineering to develop techniques for coupling models of material behavior to design software, enabling materials design to be an integral part of the global design process.

ELEMENTS OF MEANS

SOME OF THE THINGS WE WILL NEED FOR SUCCESS:

➘**MODELS AND EXPERIMENTS THAT ARE ADEQUATE TO THE TASK**

➘ **STRATEGIES FOR LINKING MODELS IN DIFFERENT SPATIAL AND TEMPORAL REGIMES - SO-CALLED "MULTISCALE MODELING"**

➘**A COLLABORATIVE, INTERACTIVE DESIGN ENVIRONMENT IN WHICH ENGINEERING DESIGNERS AND MATERIALS DESIGNERS CAN INTERACT SIMULTANEOUSLY TO DEVELOP MATERIALS AND PROCESSES SUITABLE FOR THE END PRODUCT**

➘**OPTIMIZE THE COMBINATIONS OF AVAILABLE MODELS, EXPERIMENTS AND PROBABALISTIC DATA BASES TO MINIMIZE DEVELOPMENT TIME AND COST**

MEANS Projects in Ceramic Materials

- **NOVEL SiCN CERAMICS FOR HEALTH MONITORING OF HIGH TEMPERATURE SYSTEMS; PI-R. Raj, U. Colo.**
- **MULTIFUNCTIONAL STRUCTURAL CERAMICS WITH FERROELASTIC AND MARTENSITIC TRANSFORMATIONS; PI-A. Sayir, CWRU and NASA Glenn.**

MEANS Projects in Polymer Based Composite Materials

- **MULTISCALE MODELING AND EXPERIMENTS FOR DESIGN OF SELF-HEALING STRUCTURAL COMPOSITE MATERIALS;PI- S. White, UIUC and J. Kieffer, U. Mich.**
- **INFLUENCE OF PREPREG MICROSTRUCTURE OF STRUCTURAL PERFORMANCE OF POLYMER MATRIX COMPOSITES; PI-G. Dillon, U. Pa.**
- **MODEL-BASED DESIGN FOR COMPOSITE MATERIALS FOR LIFE MANAGEMENT; PI-G. Schoeppner, AFRL/ML**
- **CURING OF COMPOSITES: AN INTEGRATED MULTISCALE PROCESS DESCRIPTION TOWARD TAILORED STRUCTURES AND PROPERTIES; PI-R. Pitchumani, U. Conn.**

MEANS Projects in Metallic Materials

- **COMPUTATONAL DESIGN OF ADVANCED AEROTURBINE MATERIALS: PI – G. Olson, Northwestern U.**
- **DEVELOPMENT OF A PHYSICALLY BASED METHODOLOGY FOR PREDICTING MATERIAL VARIABILITY IN FATIGUE CRACK INITIATION AND GROWTH: PI – K. Chan, Southwest Research Institute**
- **MICROSTRUCTURE-BASED MODELING FOR LIFE-LIMITED COMPONENTS: PI – H. Fraser, Ohio State U.**
- **DEVELOPMENT OF AN ACCELERATED METHODOLOGY FOR THE EVALUATION OF CRITICAL MECHANICAL PROPERTIES OF POLYPHASE ALLOYS: PI – P. Dawson & M. Miller, Cornell U.**

Critical Areas for Basic Research

- **Physics-based Model Development and Verification**
- **The Quantitative Description of Structure**
- **Experimental Techniques**
- **The Designer Knowledge Base**
- **Integration of Materials Models with Engineering Design**

Physics-based Model Development and Verification

"I am never content until I have constructed a … model of the subject I am studying. If I succeed in making one, I understand; otherwise I do not."

(Lord Kelvin)

Physics-based Model Development and Verification

- Models that link the behavior of materials to their microstructure must be based on the fundamental processes that determine the behavior
- Models must be expressed mathematically in three-dimensional, frame-invariant (tensorial) form
- Parameters that describe the structure of materials must be described in terms of measurable quantities expressed in tensorially invariant form
- To the extent that models contain material parameters that are not state quantities, the models must include evolution equations to account for history dependence of the parameters
- Critical experiments to verify models must be designed and performed to the extent necessary to develop a quantitative assessment of the reliability of models used in engineering design

Image-Based Models from OIM Data

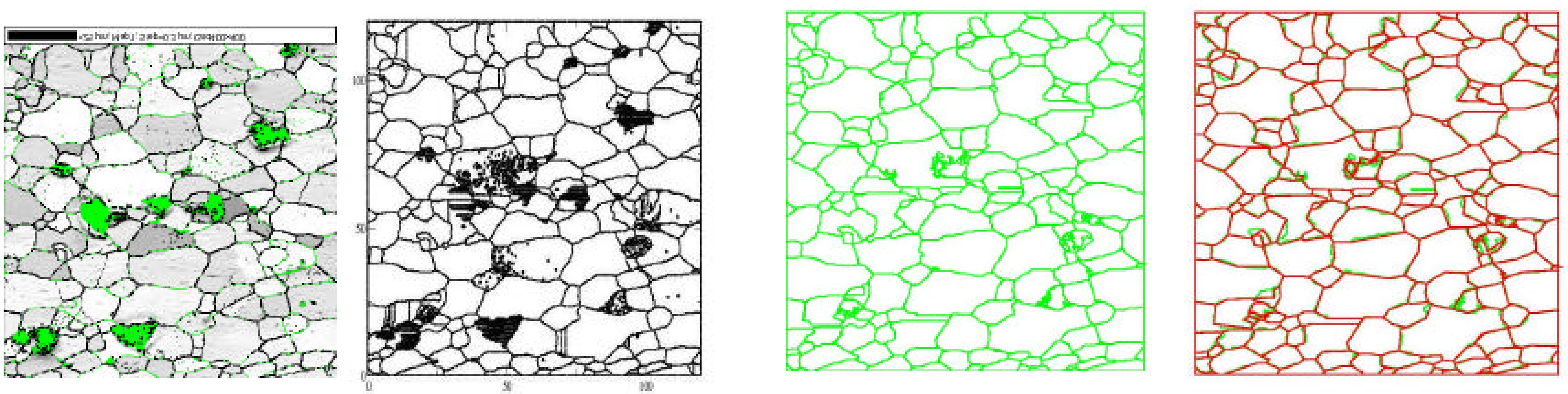
1: **Read and Filter Input Data**:

2: **Identify Grain Boundaries**:

3: Identify triple points

4: Filter the image:

5. Create Image-based elements



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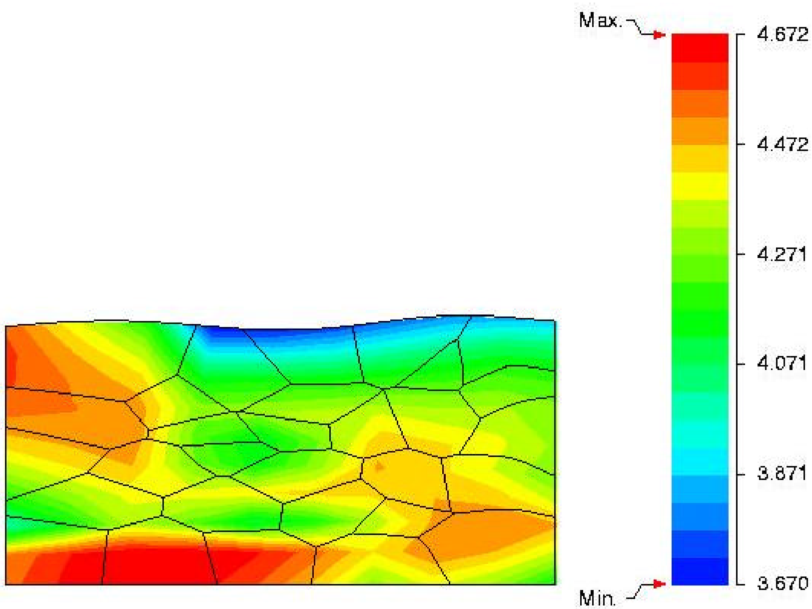
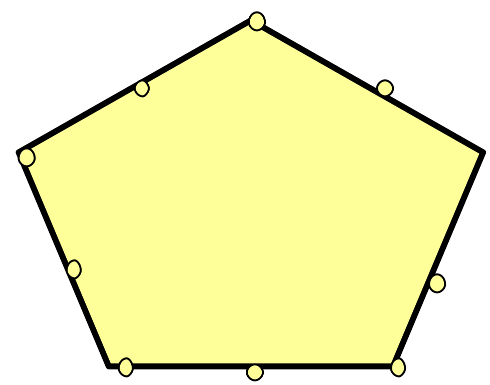
GRAIN BASED FINITE ELEMENT MODEL

- **Direct mapping of crystal topology on the FE model (each element represents a crystal grain)**
- **Element can have arbitrary number of sides**
- **Special enhanced strain formulation for strong discontinuities**
- **Grain boundaries can be facilitated with failure characteristics**
- **Trans-granular cracking can adaptively incorporated**





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RATE DEPENDENT CRYSTAL PLASTICITY

Kinematic Description

$$F = F^{*} : F^{p}$$

Slip Plane and Directions

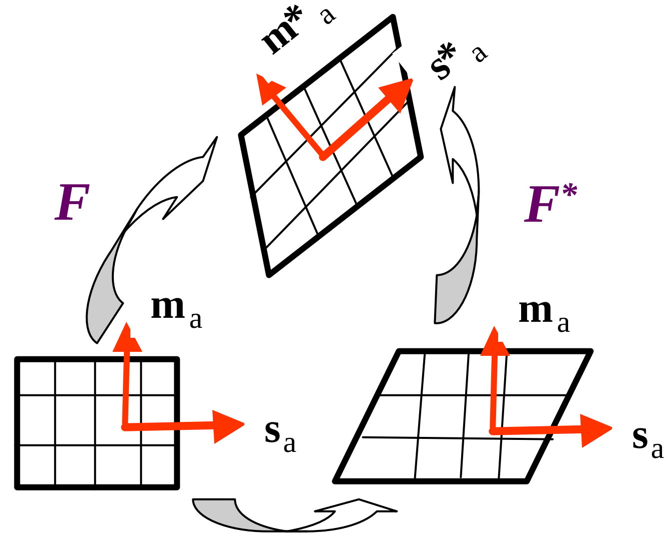
$$s^{*}_{a} = F^{*} .\, s^{0}_{a} \quad , \quad m^{*}_{a} = m^{0}_{a} .F^{*-1}$$

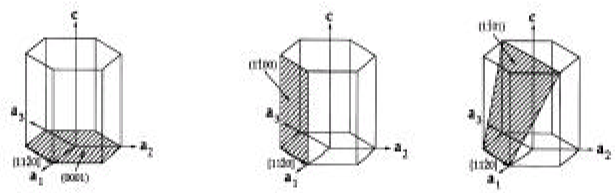
Constitutive Relations
(Second Piola-Kirchoff Stress)

$$T^{*} = \tilde{\mathbf{C}} : [\frac{1}{2}(F^{*T}F^{*} - I)]$$

Resolved Shear Stress

$$t^{a} = (\tilde{\mathrm{C}} : T^{*}).s^{0}_{a} \otimes m^{0}_{a}$$





Basal-$\langle a \rangle$ $(0001) \langle 11\bar{2}0 \rangle$, 3

Prismatic-$\langle a \rangle$ $\{10\bar{1}0\} \langle 11\bar{2}0 \rangle$, 3

Pyramidal-$\langle a \rangle$ $\{10\bar{1}1\} \langle 11\bar{2}0 \rangle$, 6

1st order Pyramidal-$\langle c + a \rangle$ $\{10\bar{1}1\} \langle 11\bar{2}3 \rangle$, 12

2nd order Pyramidal-$\langle c + a \rangle$ $\{11\bar{2}2\} \langle 11\bar{2}3 \rangle$, 6

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The Quantitative Description of Structure

"I often say that when you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind."

(Lord Kelvin)

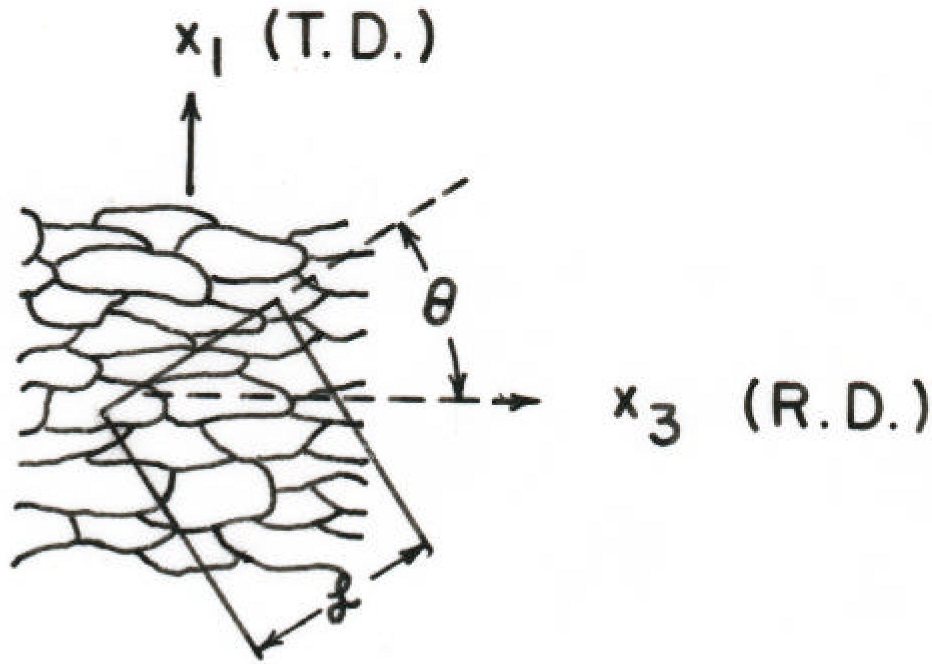
The Quantitative Description of Structure

- Quantitative descriptions of microstructure must be employed to express its crystallographic, metric, topological and inhomogeneous character in forms that can be incorporated into mathematical models of material behavior

- Experiments must be designed and conducted to determine the relationships between material behavior and the various aspects of microstructure

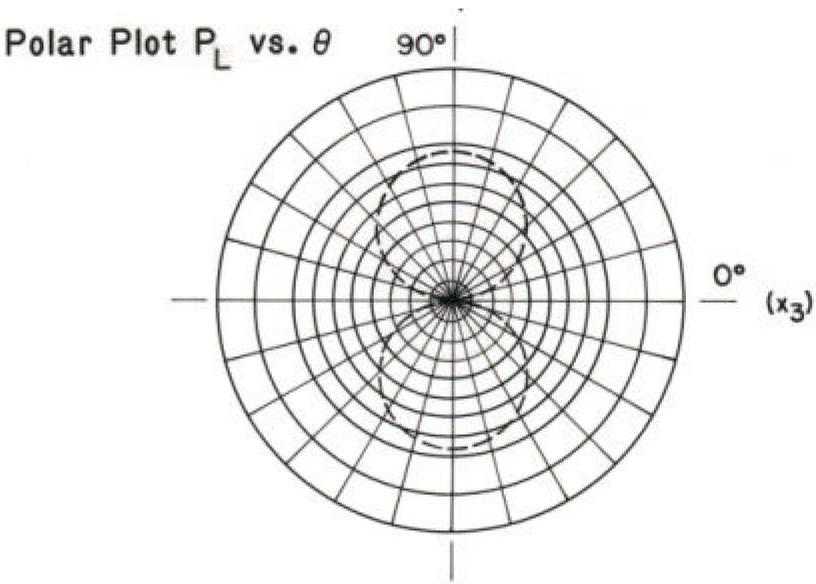
- The evolution of microstructure with thermo-mechanical processing must be modeled quantitatively to guide the development of processes that produce materials having specific microstructural characteristics

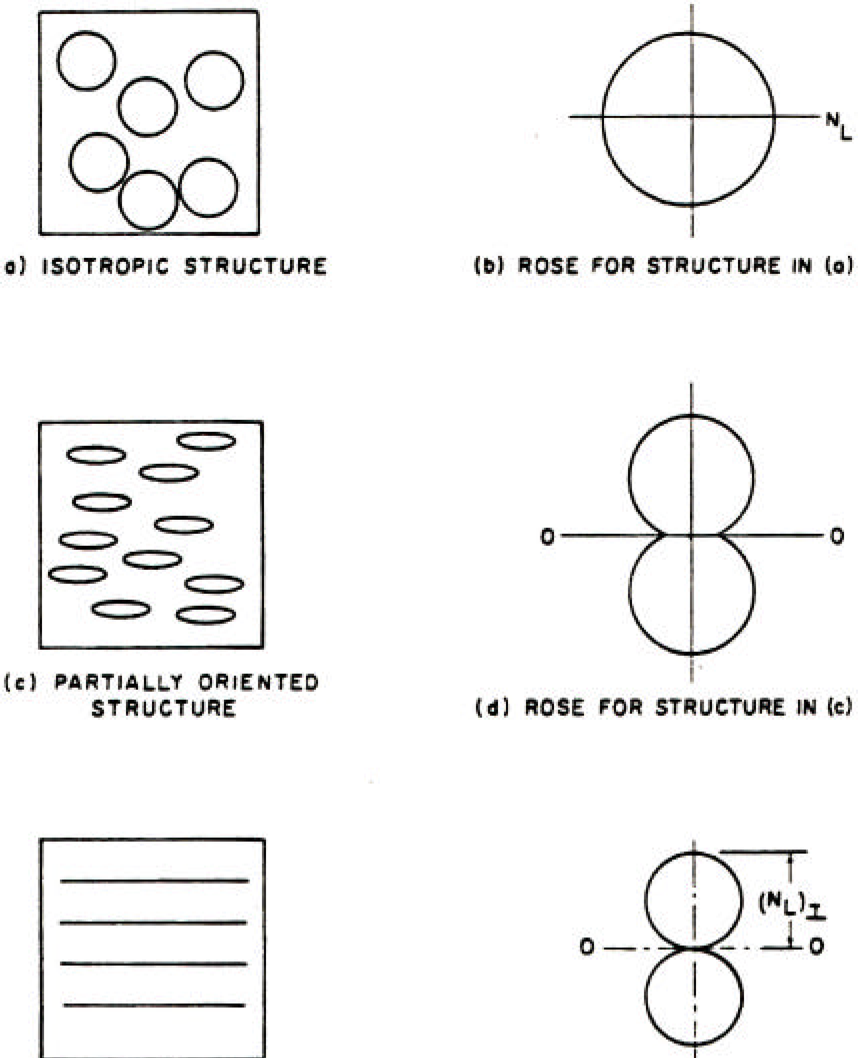
Determination of Orientation Dependence of Mean Linear Intercept



$$L = P_L^{-1} = \text{Mean Linear Intercept}$$

Rose of the Number of Intersections





(a) ISOTROPIC STRUCTURE

(b) ROSE FOR STRUCTURE IN (a)

(c) PARTIALLY ORIENTED STRUCTURE

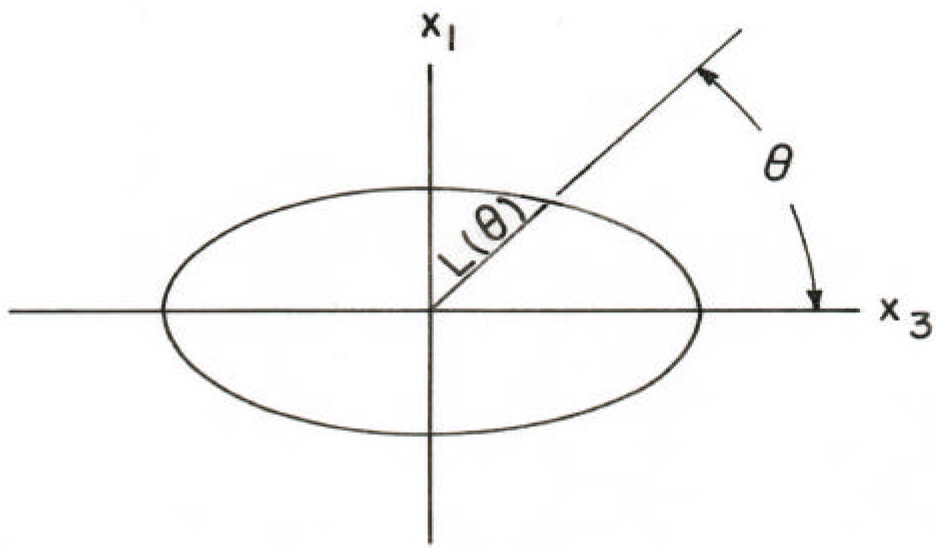
(d) ROSE FOR STRUCTURE IN (c)

(e) COMPLETELY ORIENTED STRUCTURE

(f) ROSE FOR STRUCTURE IN (e)

Fabric Tensor of Second Kind (Second Order)

Polar Plot of L vs. θ



$$\frac{1}{L} = F_{11}\sin^2\theta + 2F_{13}\cos\theta\sin\theta + F_{33}\cos^2\theta \quad .$$

Fabric Tensor of Second Kind (Second Order)

The spatial variation of P_L, the mean linear intercept of a test line in the direction of the unit vector, t, with grain boundaries, can be expressed in the form (Kanatani, 1984)

$$P_L = F_{ij} t_i t_j = L^{-1} \quad .$$

This is the expansion of P_L to second order in a Fourier series with the dyadic product, $t_i t_j$, as basis functions. Since the tensor of coefficients, F_{ij}, is symmetric, eigenvalues can be determined, defining principal axes of microstructural anisotropy.

For the cases of rolling and extrusion, it has been demonstrated that the principal directions of microstructural anisotropy are parallel to the principal axes of global total deformation in regions where the deformation is relatively homogeneous.

Experimental Techniques

" To measure is to know."

(Lord Kelvin)

Experimental Techniques

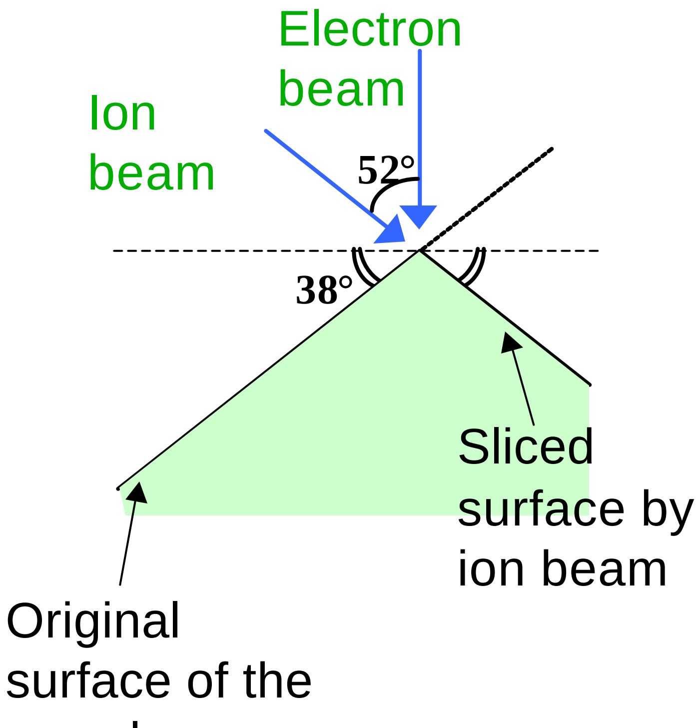
- Micro-diffraction techniques that measure lattice distortion coupled with experimental micro-mechanics techniques reveal how dislocation behavior affects deformation at the nano- and micro-scale

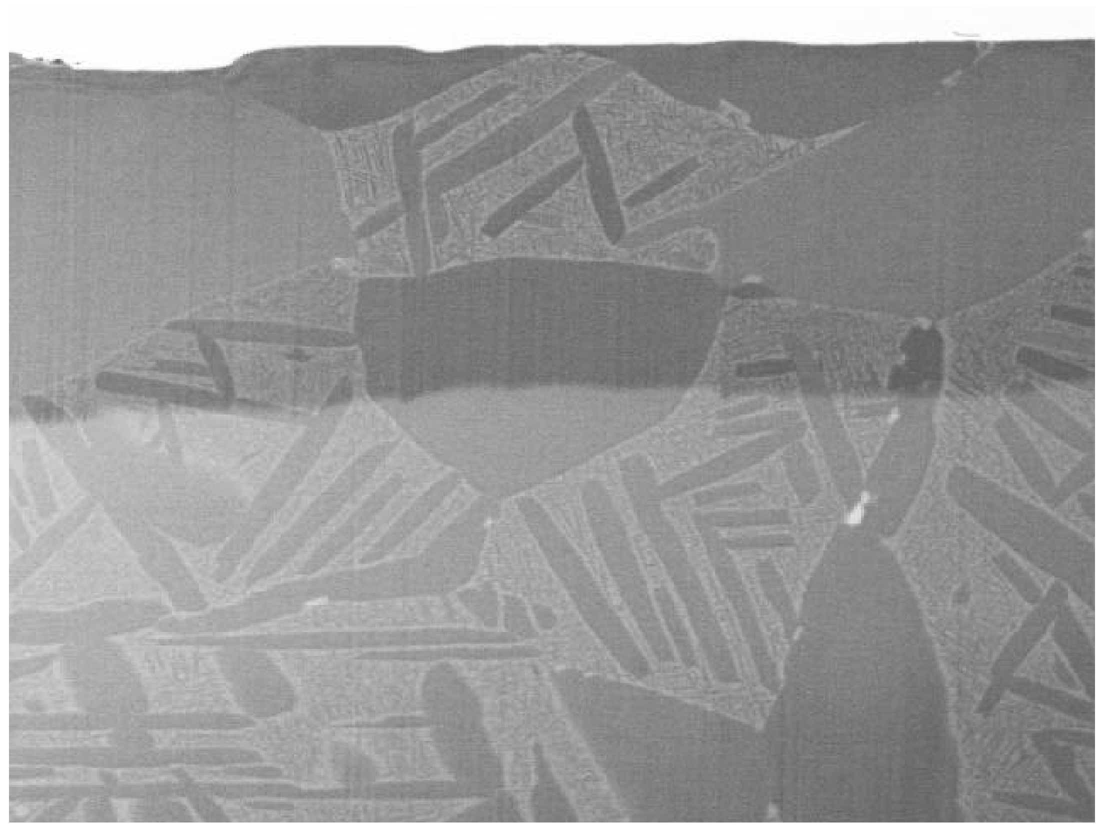
- Combinatorial analysis provides a useful screening technique for identifying composition regimes of potential interest for alloy development

- Focused Ion Beams (FIB) coupled with transmission and scanning electron microscopy provide a means of examining selected segments of microstructures with unprecedented selectivity

- Electron BackScatter Diffraction (EBSD) gives detailed information about localized distributions of grain orientations

FIB for 3-D Microstructural Representation





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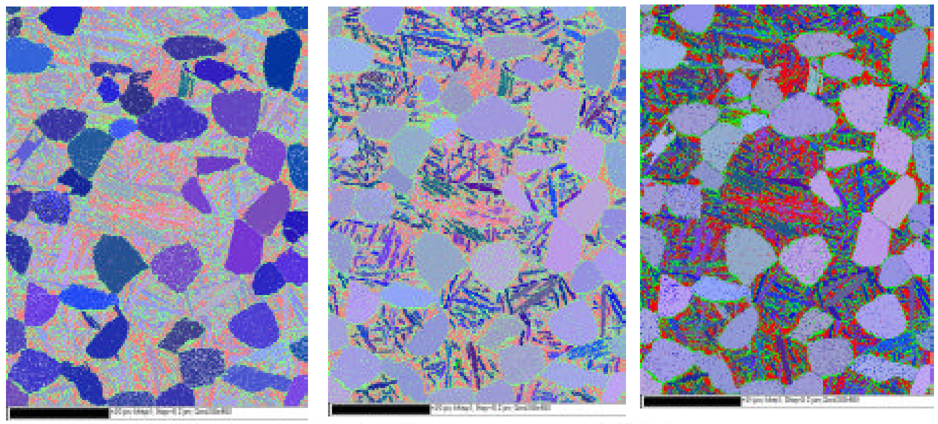
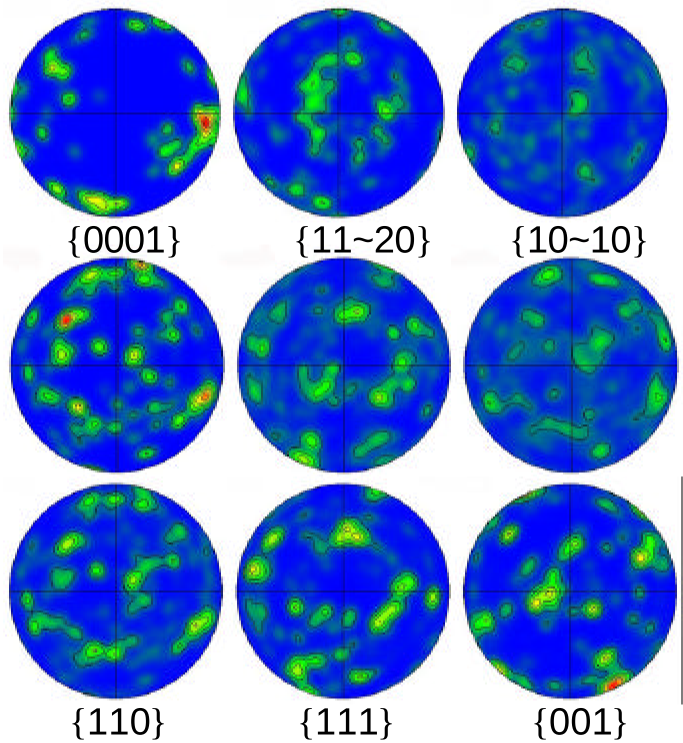
Local Texture Determination





Burger's Orientation Relationship: (0001)//{110} & <11~20>//<111>

"Equiaxed" a - **pole figures**

"Lath" a - **pole figures**

ß-phase pole figures

CAMM

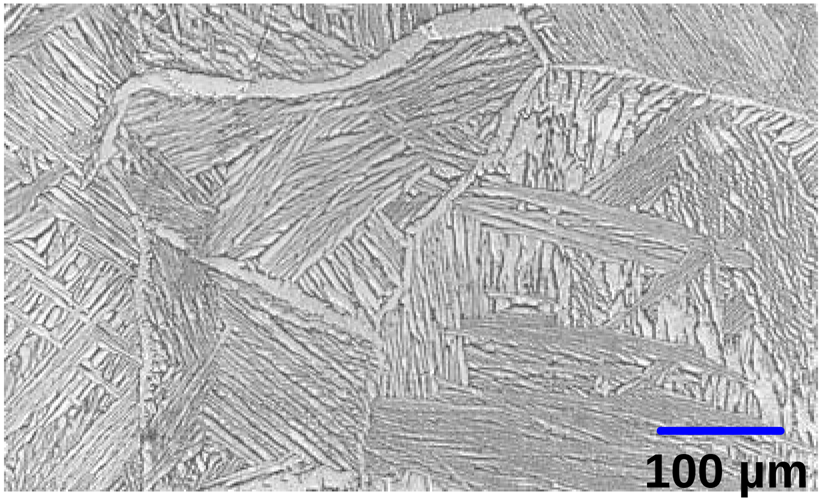
"I cannot doubt but that these things, which now seem to us so mysterious, will be no mysteries at all; that the scales will fall from our eyes; that we shall learn to look on things in a different way - when that which is now a difficulty will be the only commonsense and intelligible way of looking at the subject."

(Lord Kelvin)

The Designer Knowledge Base

- Existing information must be organized so that search methods that employ advanced techniques of information technology can be applied to extract useful knowledge
- Data must be analyzed to determine critical gaps in information in order to guide future experiments and model development
- Experiments and simulations must be conducted in a manner that the results can reveal essential functional dependencies between structure and properties
- Results of experiments and models must contain means for obtaining quantitative estimates of the reliability of predictions that use this information

Development of Neural Networks for ß-Processed Ti-6Al-4V



ß processed

***Samples processed*:**

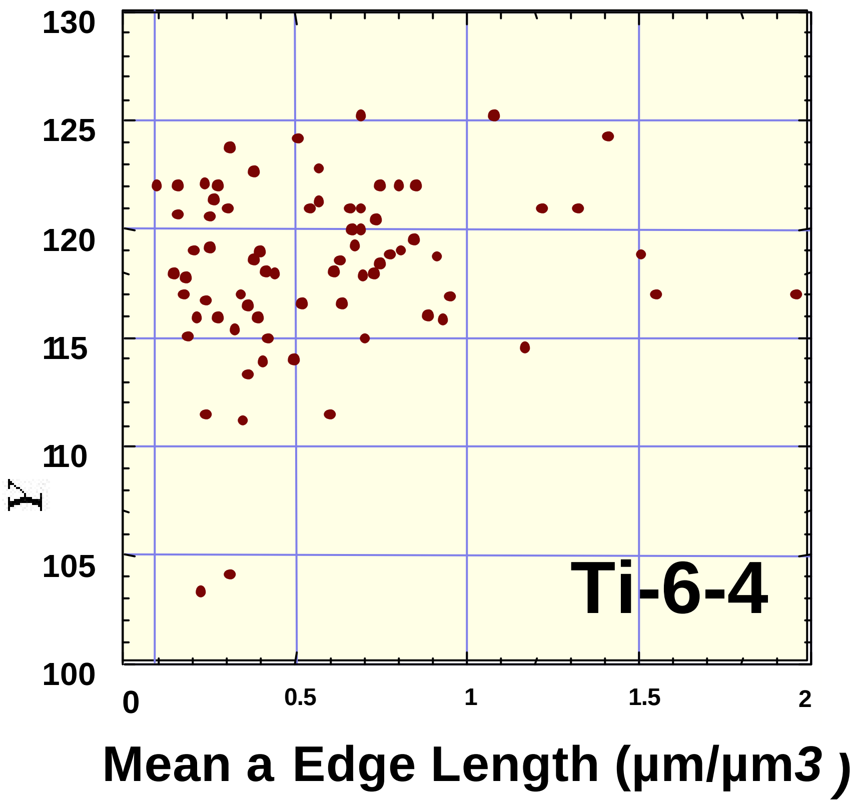
76 samples *ß*-solutionized (1050°C) and subsequently a/*ß* heated-treated over range 650°-850°C, using cooling rates of 0.3°C/s to 16.7°C/s, making use of a Gleeble TM simulator.

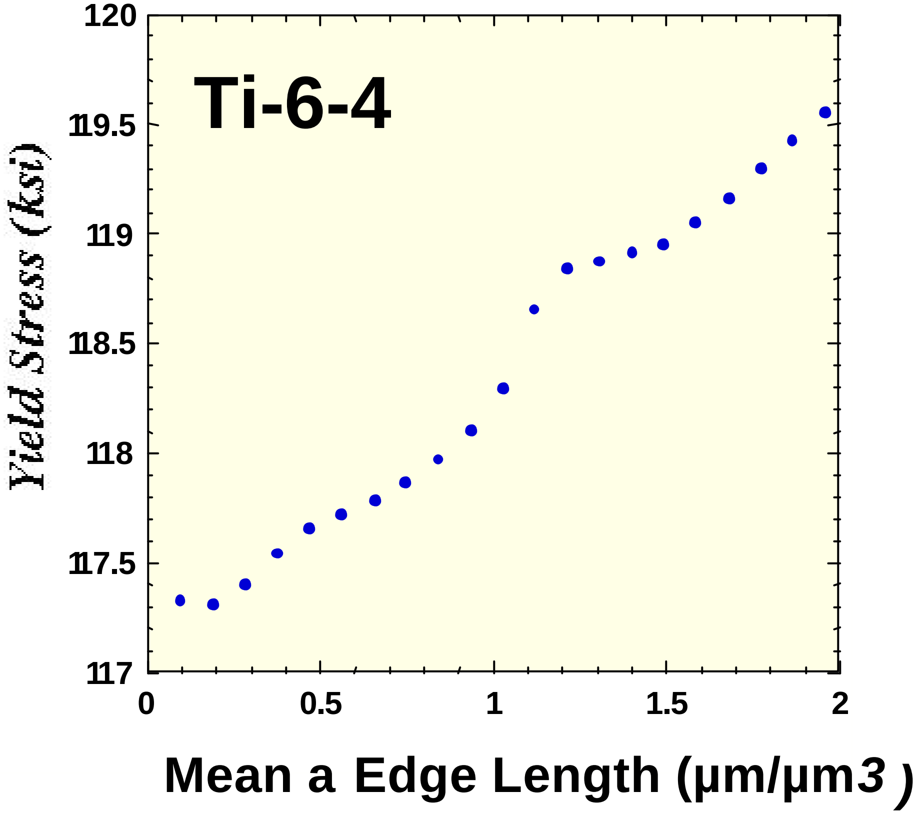
52 samples heat-treated similarly using conventional processing

CAMM

Virtual Experiment

Functional Dependence of *Mean a Edge Length* on *Yield Stress (fuzzy logic)*





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"There cannot be a greater mistake than that of looking superciliously upon practical applications of science. The life and soul of science is its practical application."

(Lord Kelvin)

Integration of Materials Models with Engineering Design

- Quantitative descriptions of microstructure must be employed to express its crystallographic, metric, topological and inhomogeneous character in forms that can be incorporated into mathematical models of material behavior
- Experiments must be designed and conducted to determine the relationships between material behavior and the various aspects of microstructure
- The design of materials must become part of the total design process

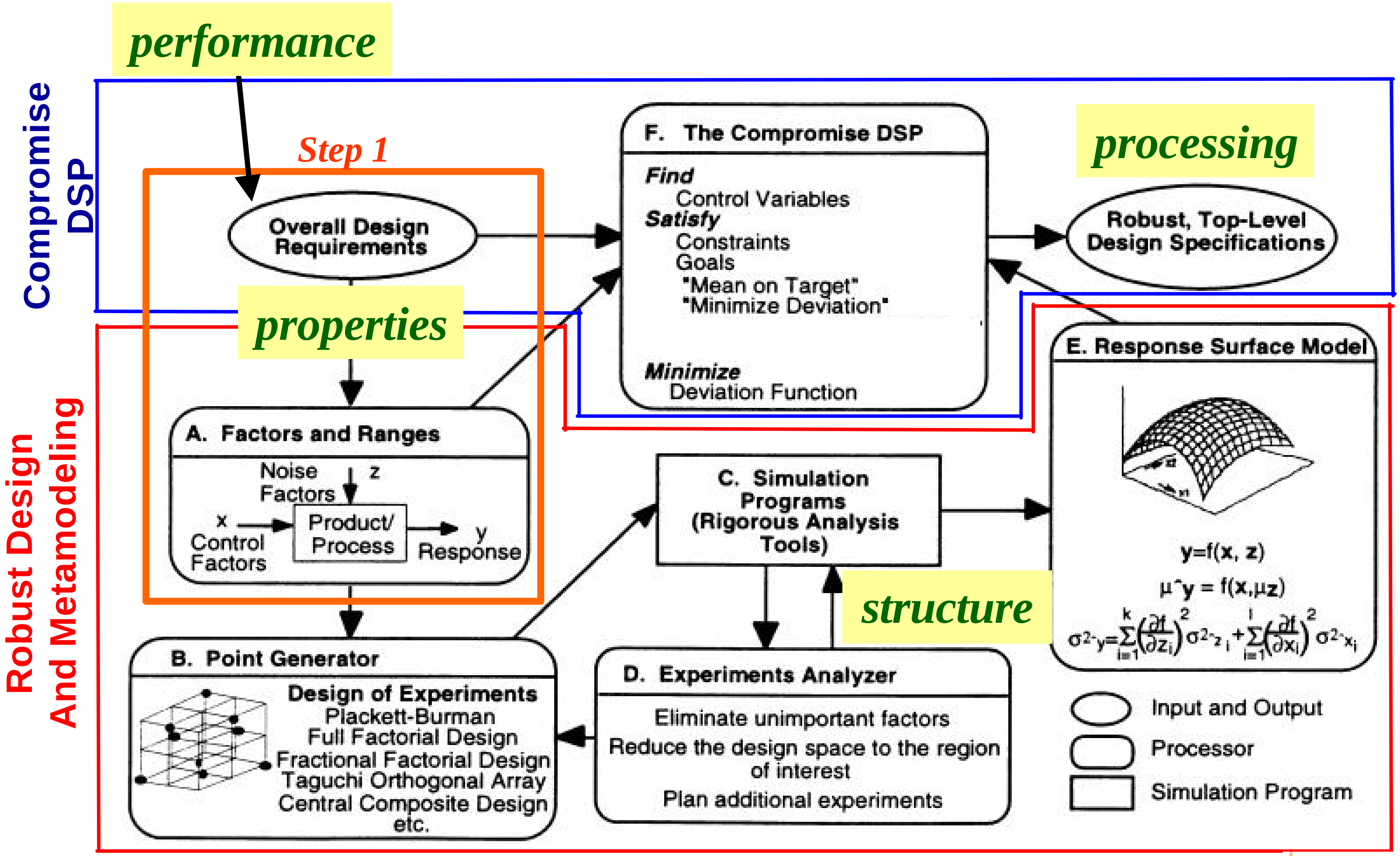
An Interactive, Distributed, Computational Environment for the Design of Multifunctional Materials and Processes

- **Multiple scales of phenomenon**
  - **Macro Scale (mm to cm)**
  - **Meso Scale (50 nm to mm)**
  - **Micro Scale (10 nm to 100 nm)**
  - **Nano Scale (0.1 nm than 10 nm)**
- **Information dependencies**
- **Hierarchical flow of information**
- **Expensive design iterations**
- **Proprietary software tools**
- **Reuse knowledge and experience**
- **Uncertainties in design variables**

- Information Management
- Management of Tasks
- Computer Infrastructure
- Knowledge Capture and Archival
- Robust Design

RCEM - Robust Concept Exploration Method

Incorporates reciprocity and hierarchy through decision-modeling interfaces



$\mu\hat{y} = f(x, \mu z)$

$$\sigma^2\hat{y} = \sum_{i=1}^{k}\left(\frac{\partial f}{\partial z_i}\right)^2 \sigma^2 z_i + \sum_{i=1}^{l}\left(\frac{\partial f}{\partial x_i}\right)^2 \sigma^2 x_i$$

Computer Infrastructure of the RCEM

“Large increases in cost with questionable increases in performance can be tolerated only in race horses and fancy women.”

(Lord Kelvin).

The Payoff

Optimal utilization of materials and processes to produce affordable, reliable and durable products for military and civilian applications.

Aim High

Interoperability is the Key to Constructive Collaboration

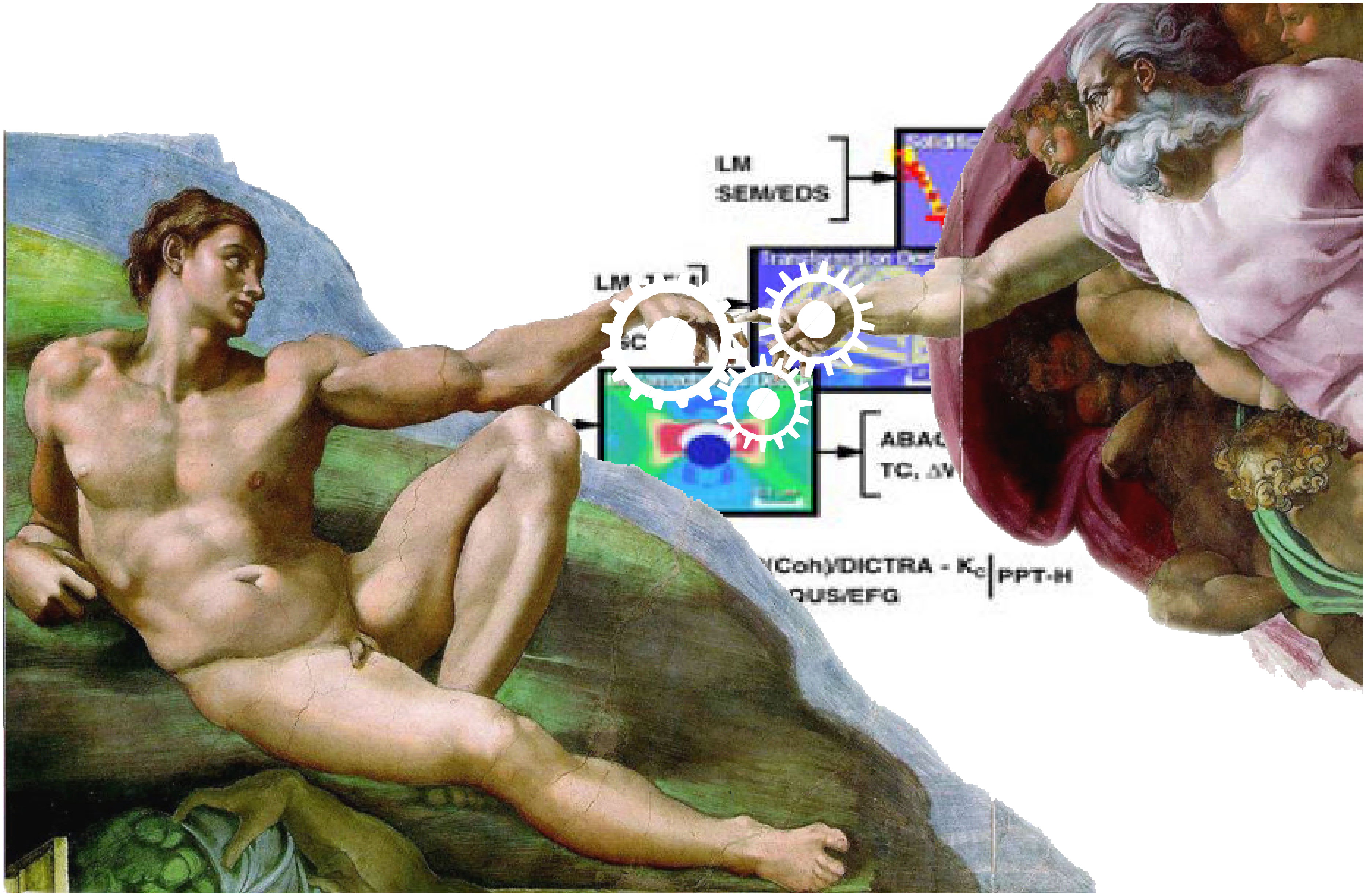
No

More

Spherical

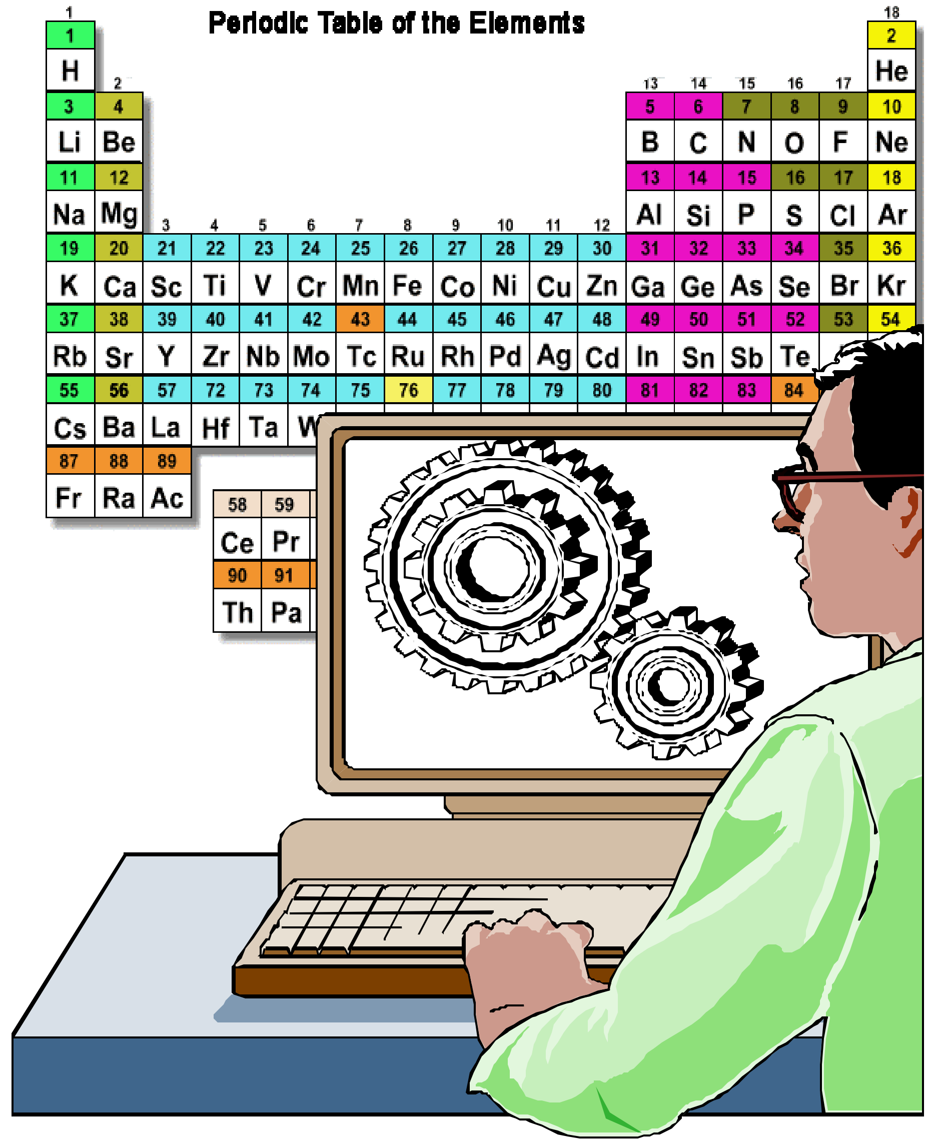
Horses

Making the Connection



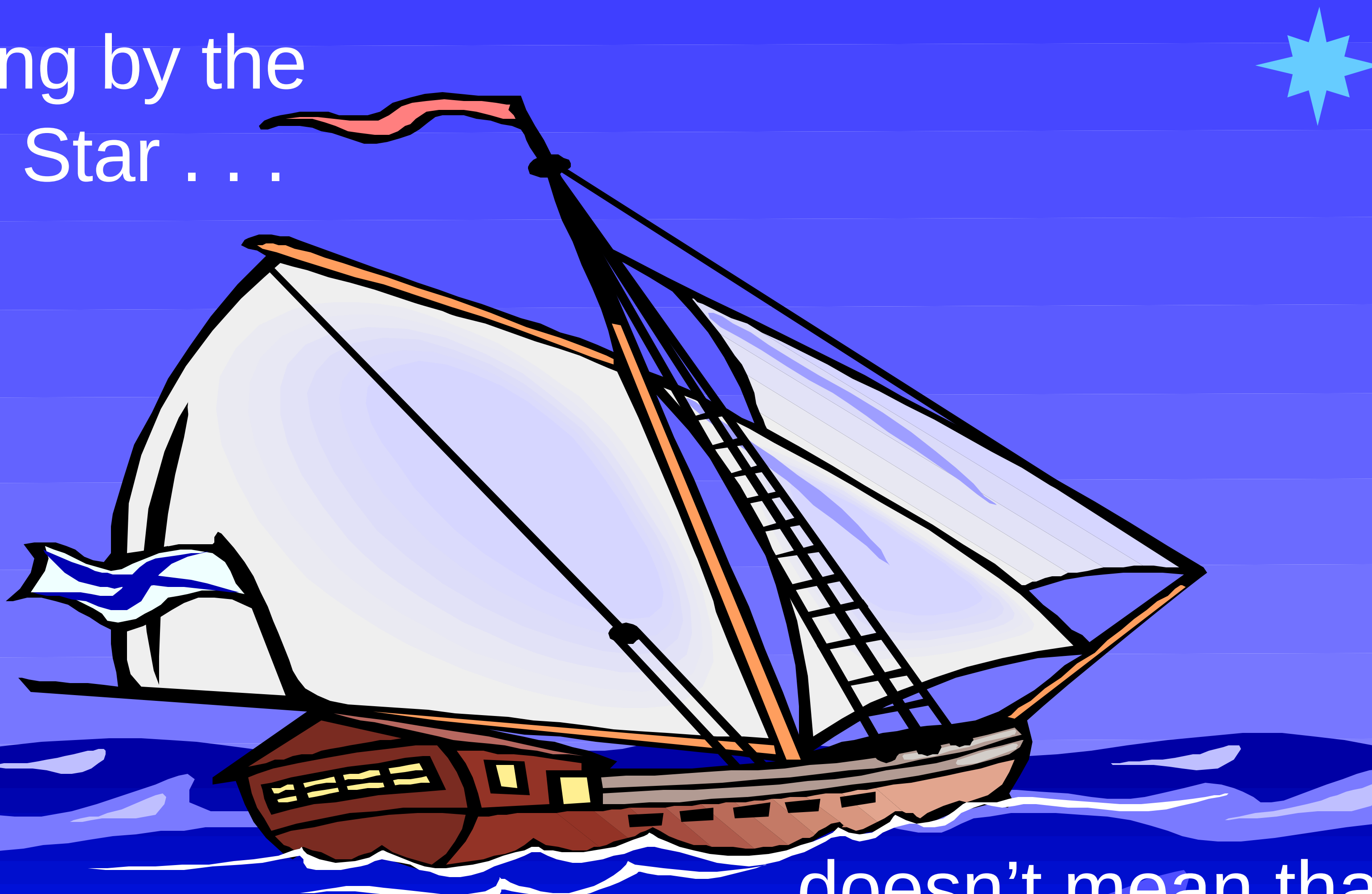
The Vision

- **Imagine that the periodic table is the ultimate data base.**
- **Construct a design space that extends from the periodic table to input into current design software.**
- **Conduct research to fill the gaps in this space.**



Following the Vision

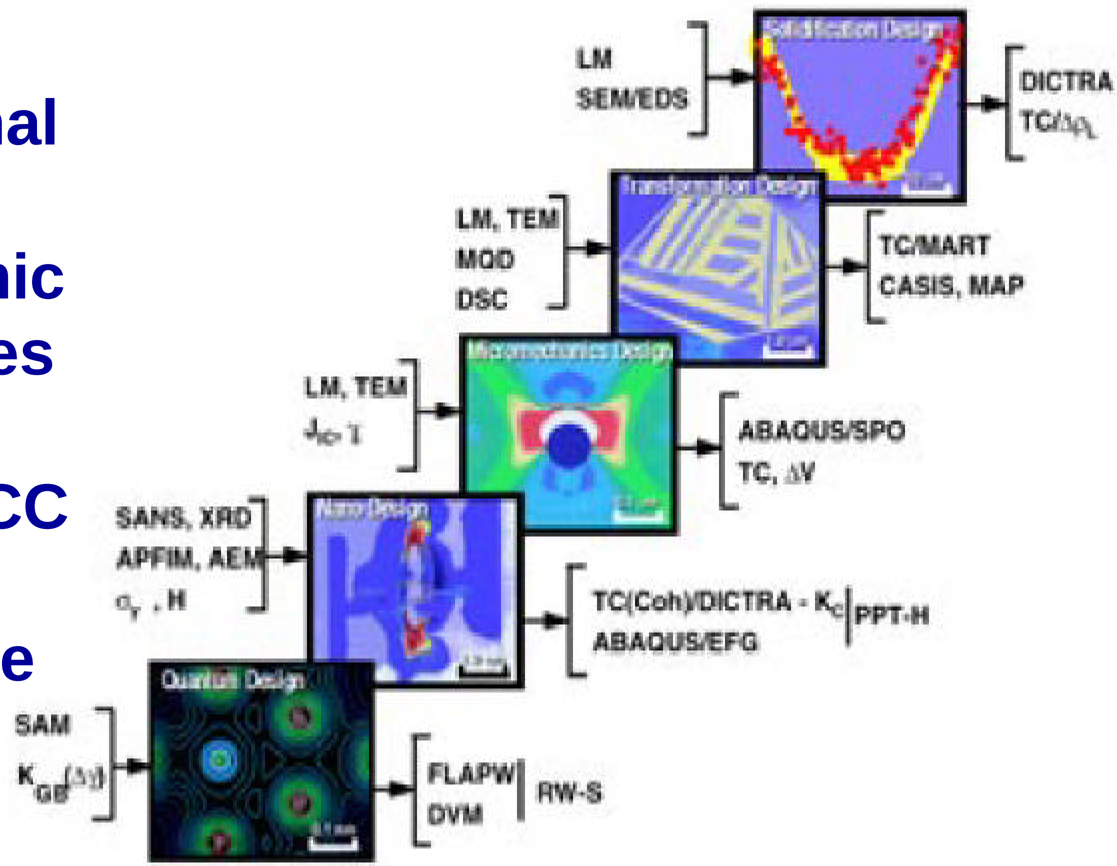
Steering by the North Star . . .



. . . doesn't mean that you're trying to go there.

Computational Design of Advanced Aeroturbine Materials (Olson, NWU)

A hierarchy of computational models will be integrated through computational thermodynamics to design a metal/ceramic system that addresses control of oxygen behavior both in a BCC Nb-based matrix as well as in stable oxide films with controlled expansion and adherence.

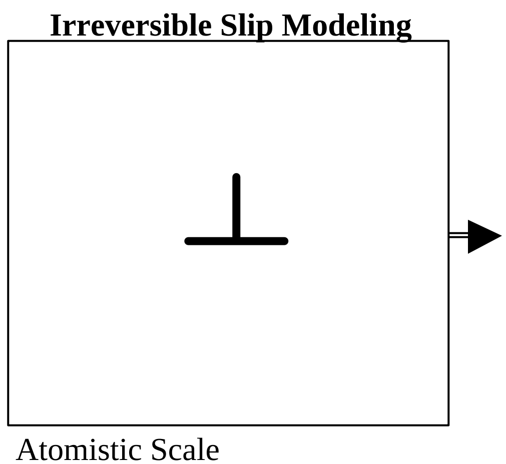


Objectives:

- To develop physics-based fatigue crack initiation and growth models
- To develop a probabilistic approach for linking physically based models into a continuum framework
- To demonstrate the utilities of the methodology in a probabilistic design setting

ATOMIC SCALE

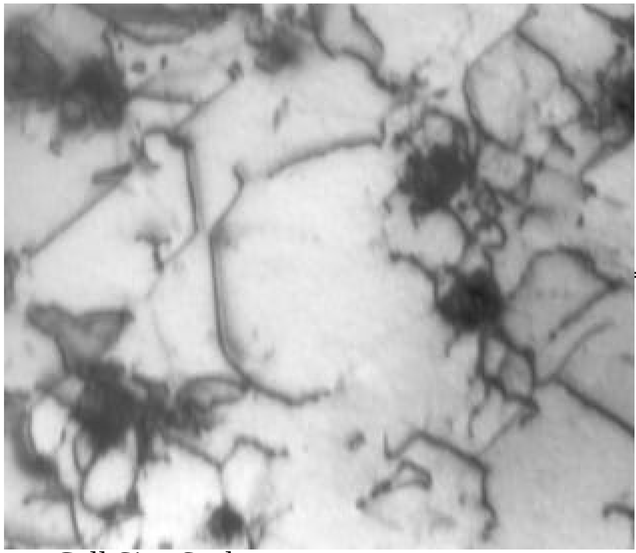
1) The friction stress for irreversible slip during fatigue will be modeled at the atomistic scale using the Peierls-Nabarro model and the thermally activated flow approach.



DISLOCATION SCALE

2) The formation of dislocation cell substructure will be modeled by considering interactions of dislocation pile-ups and cell walls at the dislocation cell size level using results from irreversible slip modeling.

Dislocation Structure Modeling

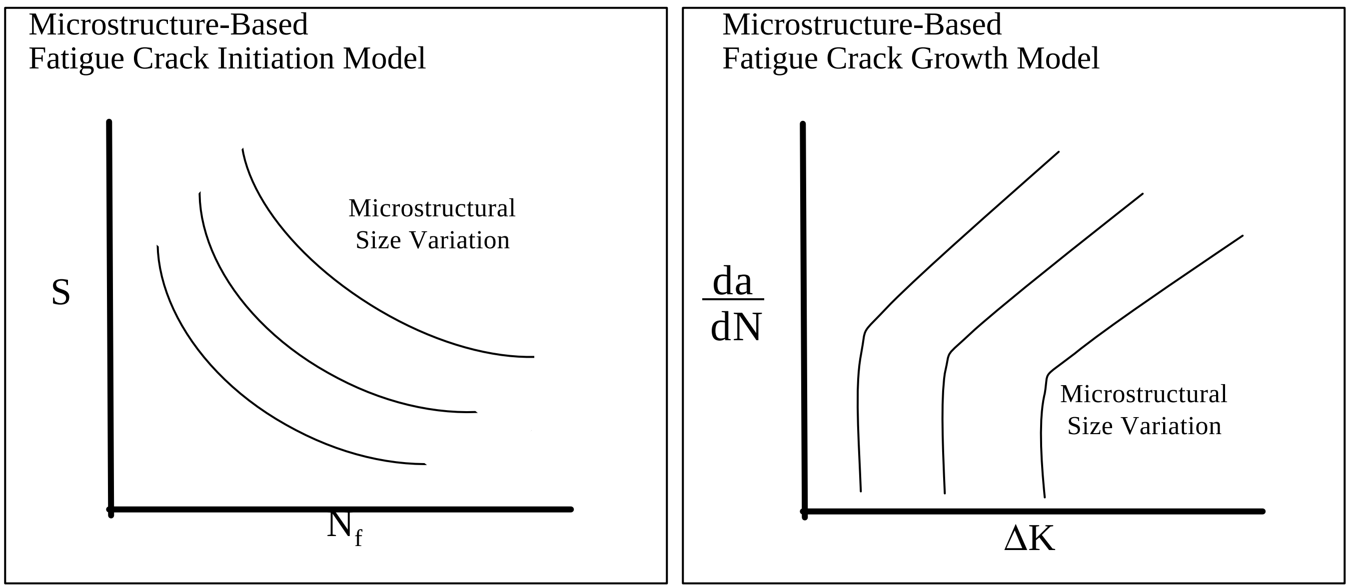


Cell Size Scale

MICROSTRUCTURE SCALE

3) Microstructure-based fatigue crack initiation and growth models will be developed at the grain level using results from dislocation structure modeling:

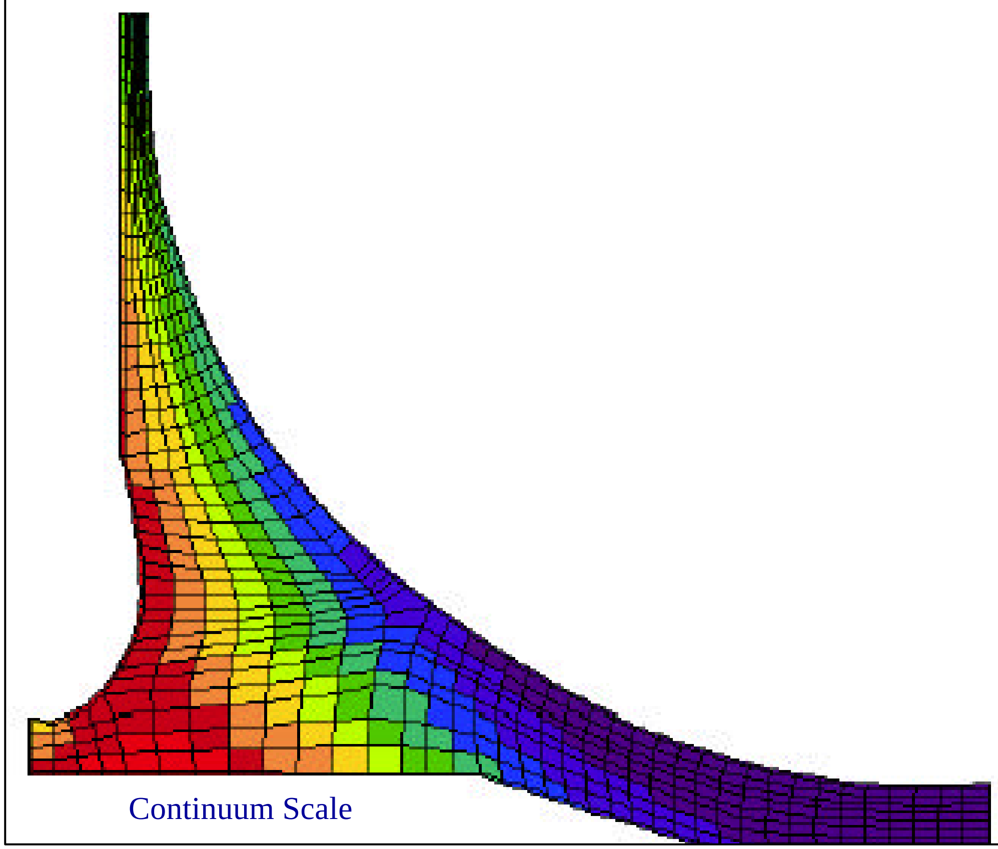
Probabilistic Fatigue Modeling



(S: Stress Range; N_f: Fatigue Life; da/dN: Crack Growth Rate; DK: Stress Intensity Factor Range)

CONTINUUM SCALE

4) The microstructure-based fatigue crack initiation and growth models will be integrated into a probabilistic framework at the continuum level.

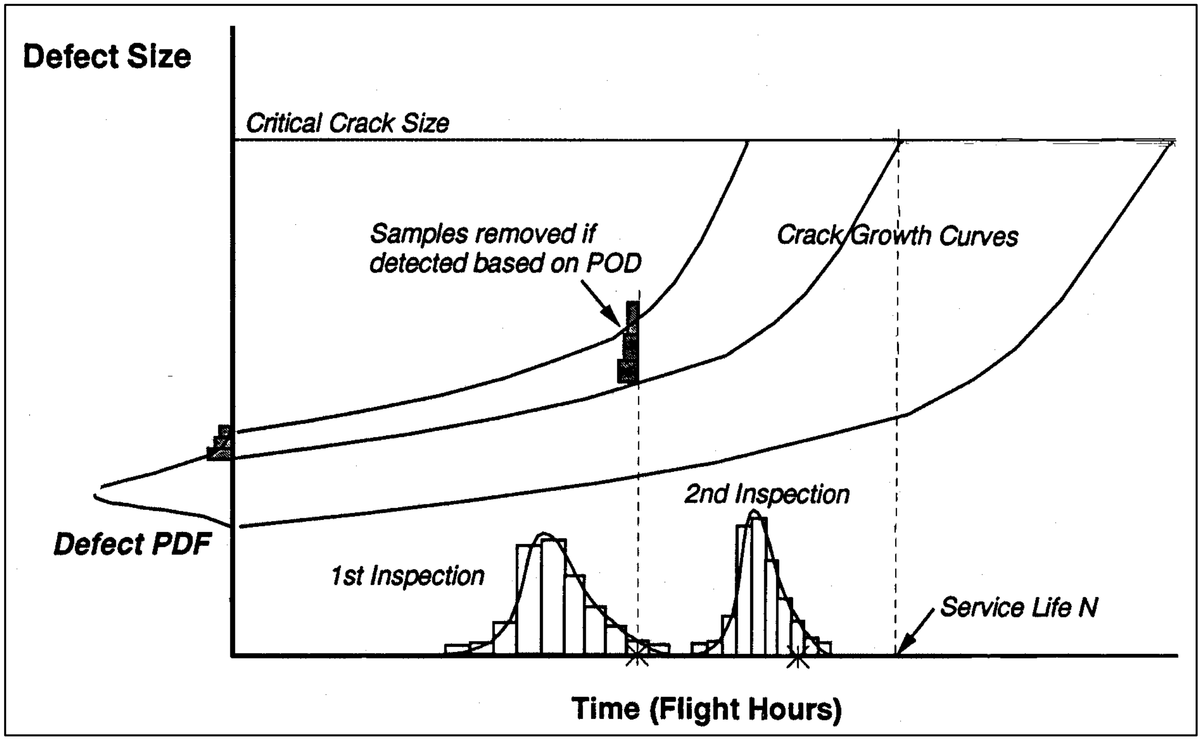


Continuum Scale

APPLICATIONS

Potential applications of the probabilistic fatigue models include component design and life-prediction analyses that include material variability and confidence limits for the fatigue properties.

Output: Probabilistic Lifetime Prediction Including Microstructure Variability

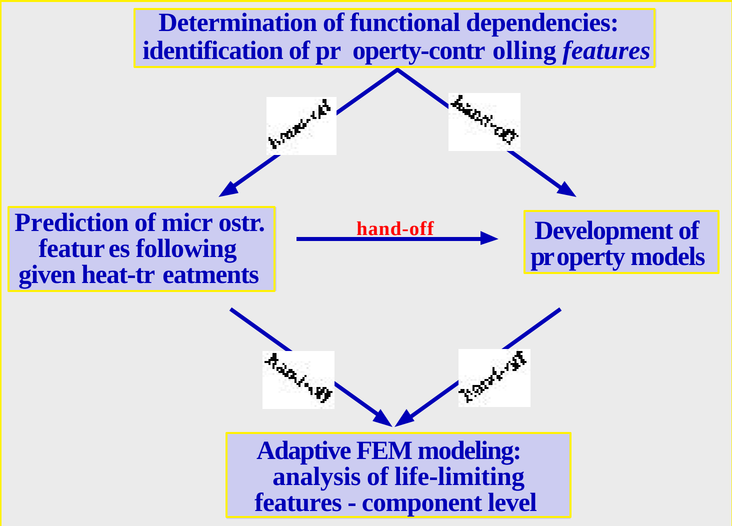


Microstructure-based Modeling for Life-Limited Components (Hamish L. Fraser, Somnath Ghosh, James Larsen*, Yunzhi Wang, James C. Williams; CAMM-OSU *AFRL)

Aims

- **The development of a set of microstructure-based models for the prediction of LCF and da/dN in Ti-6-4 and Ti-6-2-4-2**

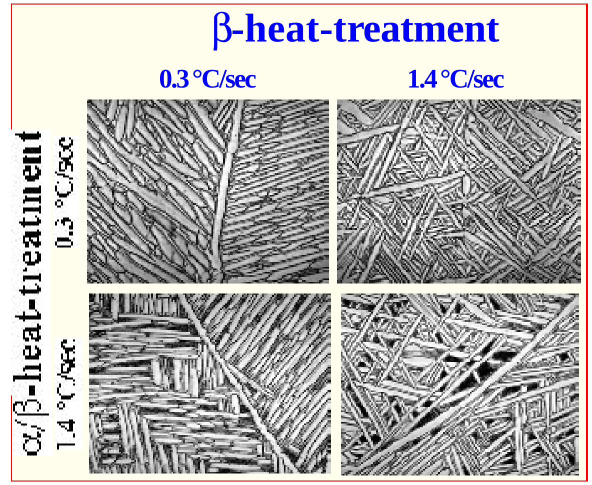
- **The provision of a set of FEM-based tools for the analysis of life-limiting features in turbine rotors**



- **A determination of the property-controlling microstructural features influencing low cycle fatigue and fatigue crack growth in Ti-6-4 and Ti-6-2-4-2**
- **The development of microstructure-based databases for the alloys Ti-6-4 and Ti-6-2-4-2**
- **A robust methodology for quantitatively determining microstructural features and their representation in modeling and simulation**

- **Quantitative simulation methodologies for the prediction of the development of microstructural features, which are key to influencing LCF and da/dN, as a function of heat-treatment**

APPROACH



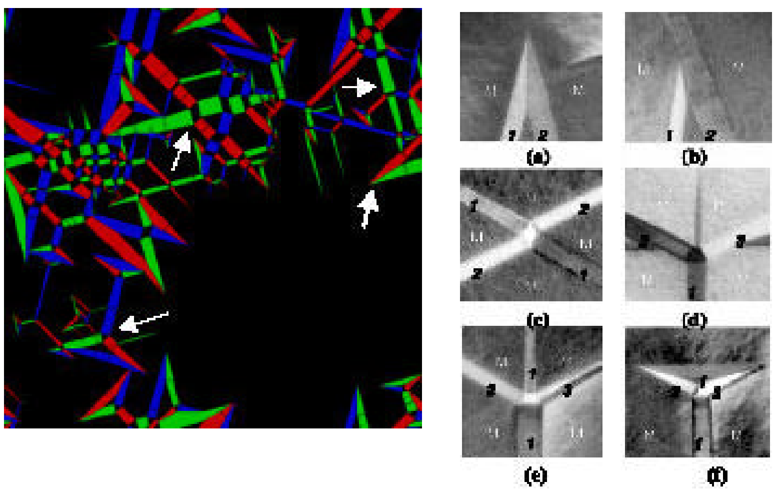
Microstructure-based Databases:

Quantitative characterization used to describe microstructure

Neural networks used to reveal functional dependencies of properties on microstructural features

Production of variations of microstructure together with property assessment provides necessary databases

This information will be used to develop physically-based models for prediction of fatigue properties



Comparison of Phase Field simulation prediction (left) with experimental observation (right, courtesy of L. Bendersky) of microstructure formed during the DO19 ✹ O-phase transformation in Ti-Al-Nb

Prediction of Microstructure Evolution:

Phase Field model will be used as the primary computational method to simulate the microstructural evolution

Modeling will include the coupling of growth to the diffusion fields of minority alloying elements, accommodation of coherency strain, and anisotropy in interfacial & grain boundary energy & mobility

Development of constitutive equations/efficient reduced-order models for grain growth and overall transformation kinetics including nucleation, growth and coarsening

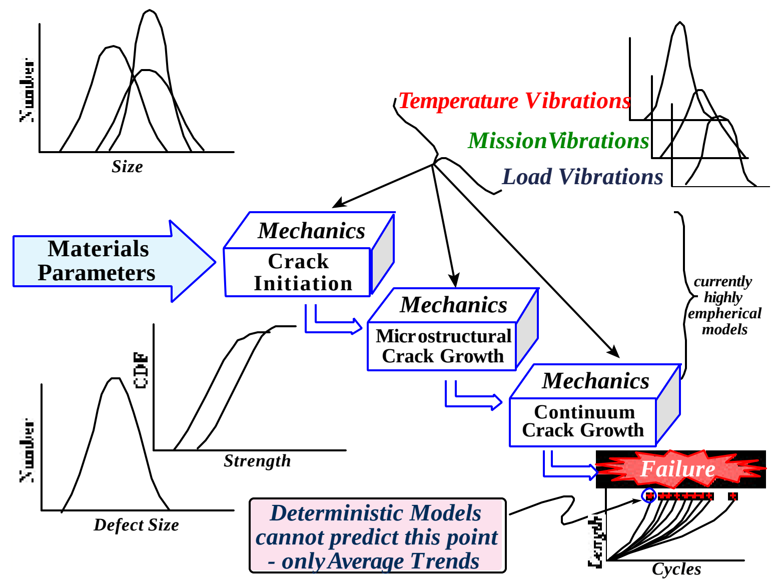
APPROACH (CONT'D)

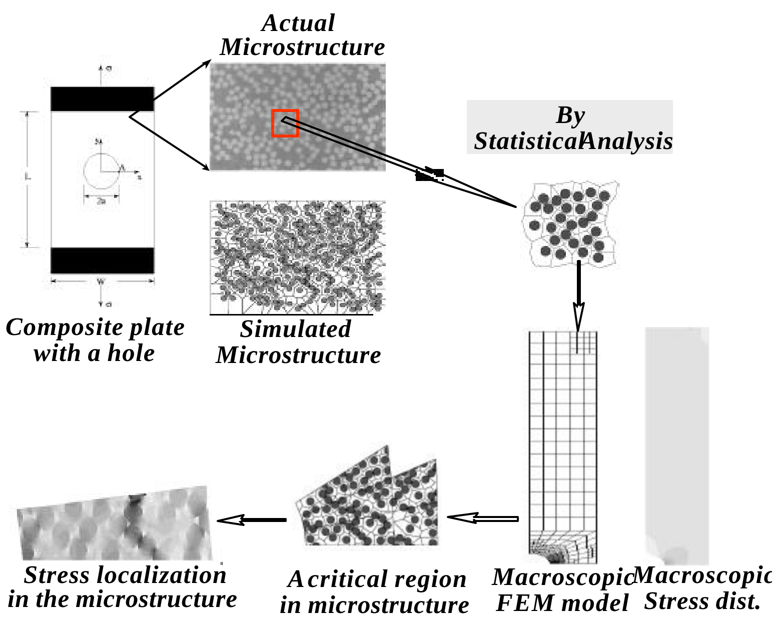
Development of Physically-based Models for Fatigue

Achieve a capability for predicting the variations in fatigue performance

Link these variations to microstructural parameters through the integration of mechanistically realistic sub-models.

Build on the neural networks relating microstructure to fatigue & crack growth rate behavior to develop physically based models





Adaptive Finite Element Modeling: Analysis of Life-Limiting Features

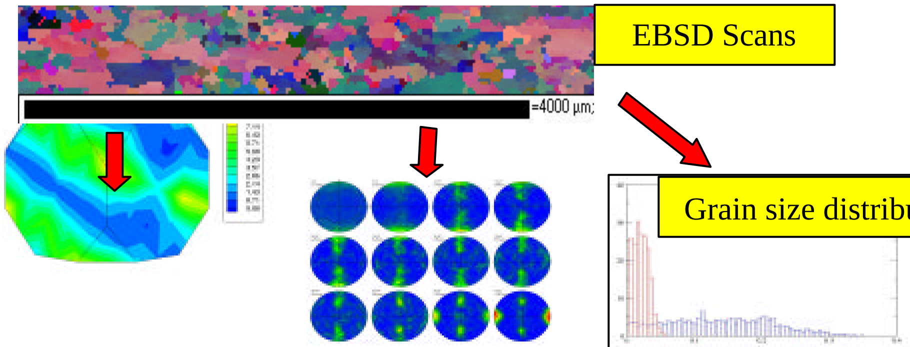
Coupled multiple scale simulation of the deformation and fracture processes of multi-colony, polycrystalline Ti alloys will be developed

The multi-scale computational system will create a hierarchy of computational sub-domains providing necessary resolution in predicting deformation and the evolution of damage and fracture

Accelerated Methodology for Evaluation Of Critical Properties in Polyphase Alloys (P. Dawson & M. Miller, Cornell U.)

- **Objectives**
  - **Rapid evaluation of stiffness and strength of polyphase metallic systems**
  - **Reduced time for insertion of alternative materials in mechanical design**
- **Methodology:**
  - **Develop protocols for a suite of simulations and experiments to assess elastic moduli and anisotropic yield surfaces**
  - **Deploy around the Digital Material framework**
  - **Interface required diagnostic tools via the Digital Material**
- **Diagnostic Tools:**
  - **Simulation: grain-by-grain finite element models of polycrystals**
  - **Experiments: mechanical tests and *in situ* diffraction measurements**
  - **Visualization: advanced graphics as interpretation aids**

The Digital Material
(P. Dawson & M. Miller, Cornell U.)



EBSD Scans

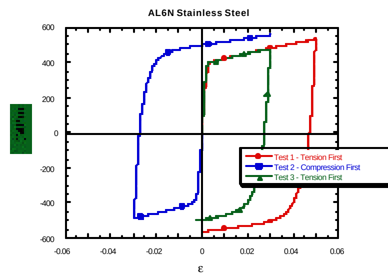
Grain size distributions

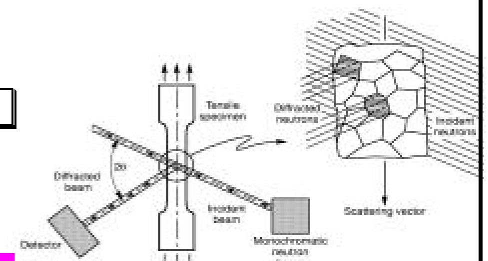
ODF

MODF

Characterization Experiments

Conventional Tests

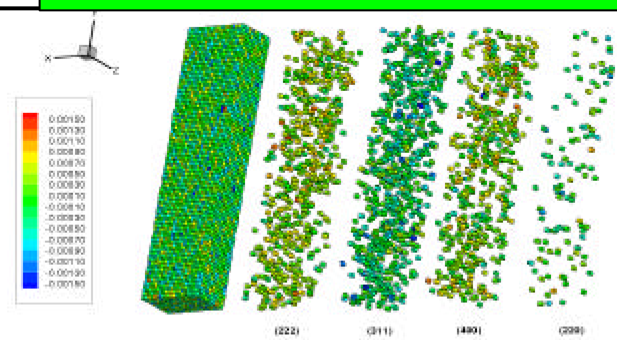




Mechanical Tests

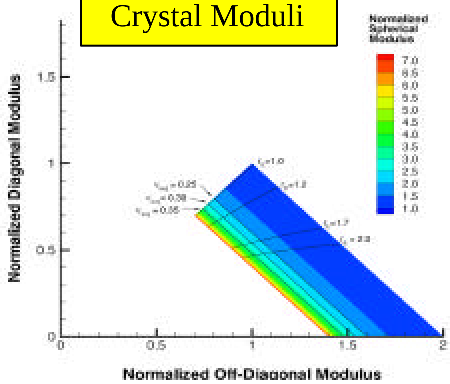
In-Situ Neutron Diffraction.

Simulate response of polyphase aggregate



Numerical Tools

Crystal Moduli

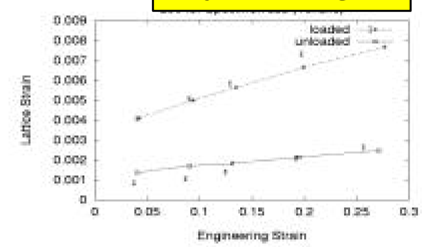


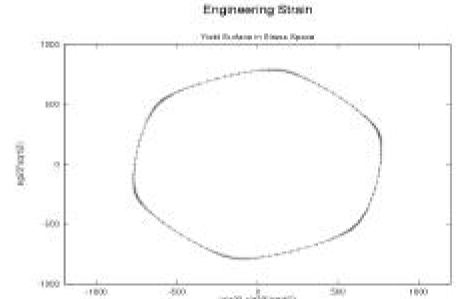
Stiffness

Determine single crystal moduli

Determine slip system parameters

Crystal strengths





Strength

Yield Surface

The Digital Material – Construction and Application