Some Possibilities for MEAN Ceramic Systems

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Scope

ML Ceramics Group viewpoint of topics in ceramics that seem suitable for computational intensive approaches.

Includes topics on which we haven't the wherewithal to collaborate, though we are happy to consult.

May include topics of little interest to the AFOSR PMs responsible for source selection.

Ceramics Research in the Materials Directorate

- Robust Continuous-Fiber Ceramic Composites
  - Environmentally resistant interface property control
  - Composites based on oxide fiber-coatings
- Component Targeted Design
  - Thermal stress resistant hybrids
  - Tailored architectures
- Basic Properties Germane to the Above
- Basic Properties Potentially Enabling for New AF Applications

Topics

- Tools for Efficient Maturation & Application of Ceramic Composites

- Phenomena Amenable to 1st Principle Treatment

Goals for Insertion of CMCs

- Put them where they provide real advantages
- Don't put them where they don't
- Anticipate what the emerging issues will be and address them before they become critical, to wit…
- Use the properties, but…
- Avoid disastrous surprises
- Discern what is necessary to simultaneously scale material capabilities, experience base, design tools, and infrastructure for viable economics

Ceramic Composite Technology

Where We Are Now

- Clear T advantages
- Clear proof of engineering potential
- Marginal lifetimes for many applications
- Simple small shapes
- Limited n-D ability
- Evolutionary processes
- Limited infrastructure and high costs
- No business base

Where We Need to Go

- Clear T, t advantages
  - Better life, not just better life prediction
- Properties in shapes
- Attachment “palette”
- Statistically Known Processes
- Reliable properties
- Real applications & businesses
- New Design Philosophy
  - Integrated Material/Component Design
- New Design Tools
  - AIM-like approach

Design with Ceramic Composites

- With metals it is feasible to have nominal properties at any location in a part
- With CMC, better to recognize there are no nominal properties…
  - Characteristic of the **local** architecture & microstructure
  - Hence a characteristic of the part, not the material
  - Therefore properties must be locally designed
    - But this is as much an opportunity as a problem
- Why not carry further to more fully tailor to the application?
  - Most CMC parts in large thermal gradients so…
  - Graded E, CTE, etc… can be beneficial
  - Hence Hybrid CMC/Metals, CMC/OMC

What's Needed for Intelligent Design and Application of CMCs (1/3)

- Complex-architecture preform processes
- Processes for precision fiber placement
- Processes for fiber-coating in complex preforms
- Processes for controlled matrix microstructure – including designed void distributions
- Processes for infiltration of complex archs

What's Needed for Intelligent Design and Application of CMCs (2/3)

- Tools for design/prediction of local properties
  - Meso-mechanics: between micro and e.g. laminate mechanics
  - Variable RVEs (Representative Volume Elements)
- Integrated Material/Component Design
  - Design tools integrated with mesomechanics models / local property prognosticator
- Tool for translating local architecture into weavable macro-architecture
- Tools for optimizing design for local properties and local loading
- Effects of constituent and microstructure variability on properties

What's Needed for Intelligent Design and Application of CMCs (3/3)

- Integrated designs for hot structure
  - Integrated materials technologies
  - Hybrid designs for non-parasitic, optimal material selection
- Efficient database and robust models for full-life modeling.
- Lifetime Design
  - Best lifetime balance of properties
  - Graceful retirement
    - Smart function, diagnostics, prognostics

Focus of Complex Architecture / Hybrid Composite R&D

OMC

Existing industry and applications

Potential near-term benefit

Available data bases and baseline experience

CMC

Smaller more complex components – greater ultimate benefit

Design for thermal stresses critical – hybrids potentially more important

Early in development – can build from the beginning

Initial focus on architecture will benefit both

AIM: Metals

(AIM = Accelerated Insertion of Materials)

- Great width and depth of experience
- Large data bases
- Critical defects are known
- Critical behavior is well understood
- Viable businesses exist and are independent of AIM…
- …but provide users and user-pull
- Metals ideal for <u>developing</u> the AIM methodology

AIM: Ceramic Composites

- Very limited experience
- Minimal data bases
- Major critical factors are understood, but
- More subtle effects in long service are unknown
- Viable businesses mostly do not exist; could be strongly affected by AIM
- Limited users, so limited user-pull
- AIM CMC could dramatically affect introduction and application philosophy of CMC
- …and the very nature and capabilities of future systems
- Ceramic Composites are ideal for <u>exploiting</u> AIM methodology

AICerC: Summary

Advantages of AICerC

- Real Impact on insertion of a new technology
- Ground-up AIM methodology

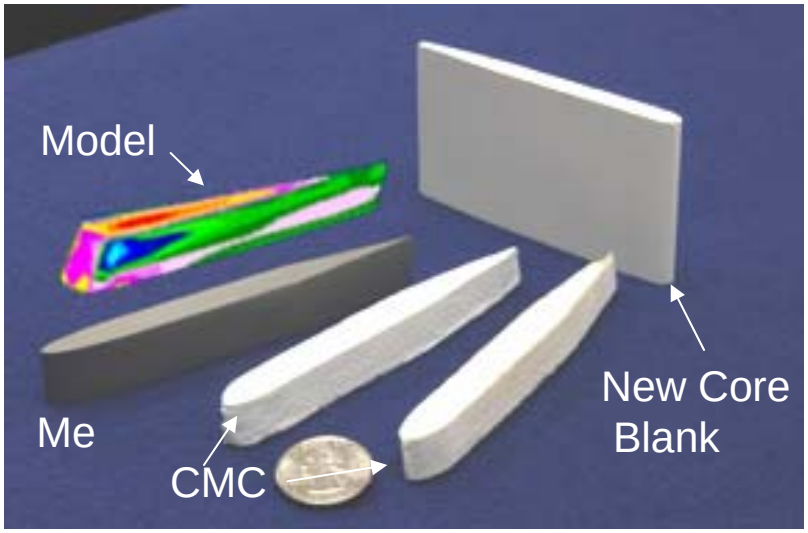
Hazards of AICerC

- A few remaining technical loose ends
  - Limit breadth and focus of CMC applicability
  - Could derail higher payoff targets
  - Could delay / derail / limit impact of AICerC
- Limited existing industry, credible partners

AFOSR MoM/ML Task: Targeted Material Design

Objective :
Provide the key science for development of new ceramic routes to superior systems

Current Primary Goal:
Intelligent design of hybrid composite materials with features targeted to address the most problematic aspects of aggressive applications.



UC3 Turbine Vanes

Approach:
Develop tools for concurrent material/structure design and use to develop tailored designs for optimal performance in specific environments

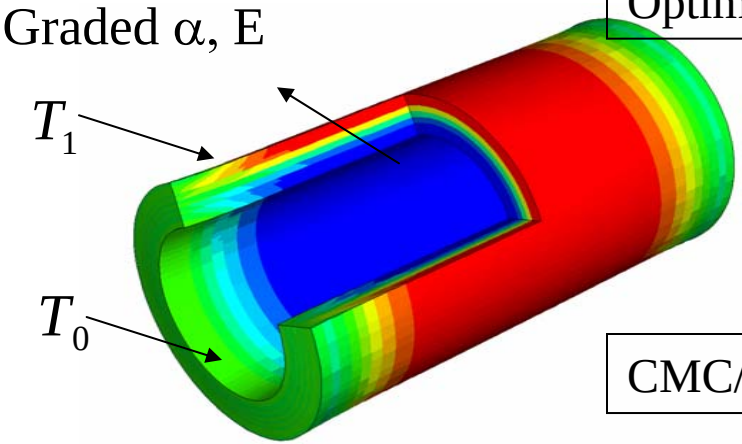
Payoff to Air Force:

- More efficient, durable, stealthy and clean turbine engines
- Higher performance, more durable rocket and space propulsion
- Higher T, more durable and stealthy hot structure for rapid access to space

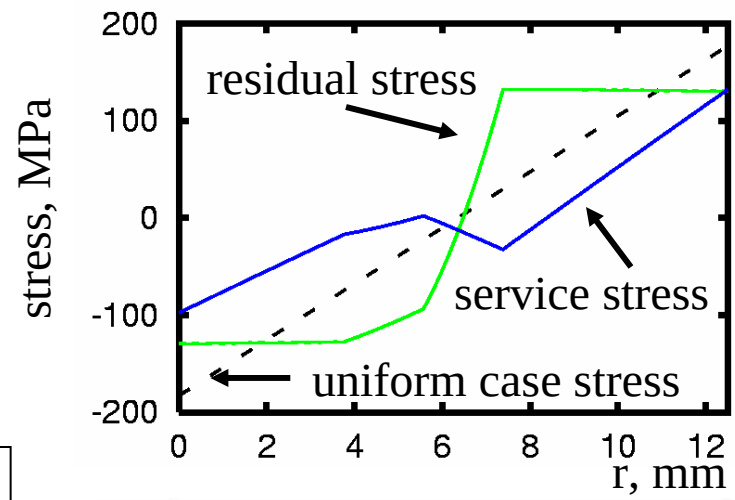
Hybrid Composites
For Thermal Stress Control

Hybrid composites comprise 3 or more structural elements tailored to component function and environment. Here CTE is varied to reduce in-service thermal stresses.

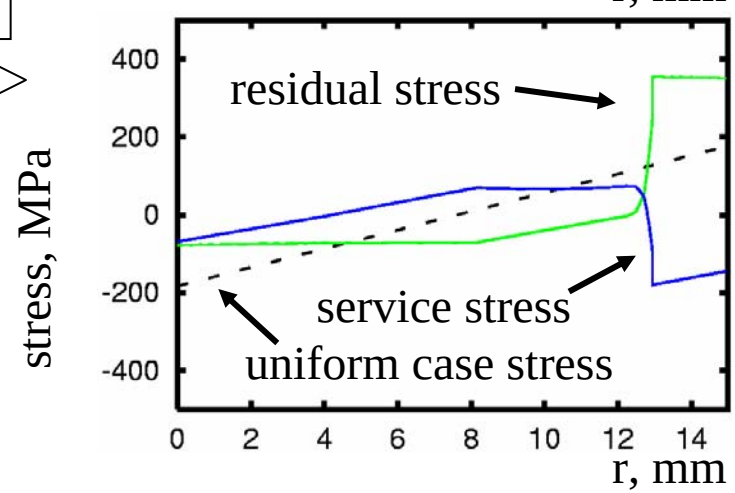
Graded α, E



Inverse Solution for Optimized α



CMC/Ni alloy Hybrid



Hybrids are designed to:

- moderate material selection compromises
- match the properties to the local requirements
- distribute stresses in the most favorable way
- can be N fibers in M matrices + monolithics

Topics

- Tools for Efficient Maturation & Application of Ceramic Composites

- Some Phenomena Amenable to 1st Principle Treatment
  ML not active in many of these: could consult, but limited ability to collaborate

Some Phenomena Potentially Amenable to 1st Principle Treatment

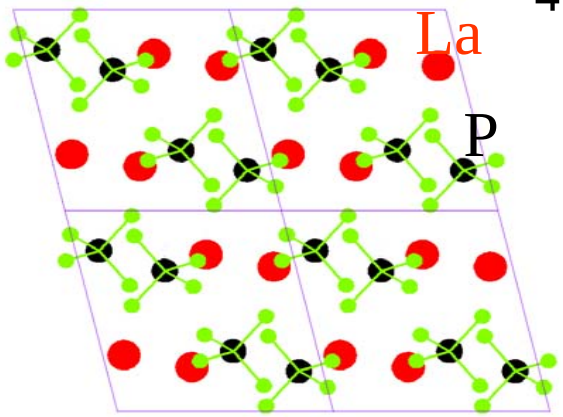
- Properties of mixed oxides & carbides
- First principle predictions of refractory hydrophobic oxides for e.g. TPS
- Modeling oxidation of UHTCs in reentry environments - monotonic oxygen, plasma, free radicals, etc.
- Corrosion-assisted crack growth
- Phase/Grain Boundary Strength in Oxides
- Segregation Effects on Boundaries
- Dopants in YAG (for lasers)
- Dopant Effects on Creep of Oxides
- Properties and Stability of HT Amorphous Materials
- Lead-free, high strain piezos

A Possible Approach

- **1st-Principle model predicts basic crystal properties**
- **2nd level model predicts eg twinning/piezo/SCC behavior and designs experiments**
- **Experiments "vet" the modeling, provide iterative feedback**

Example Topic from AFOSR Ceramics / ML Task: Deformation in Refractory ABO_4 Oxides

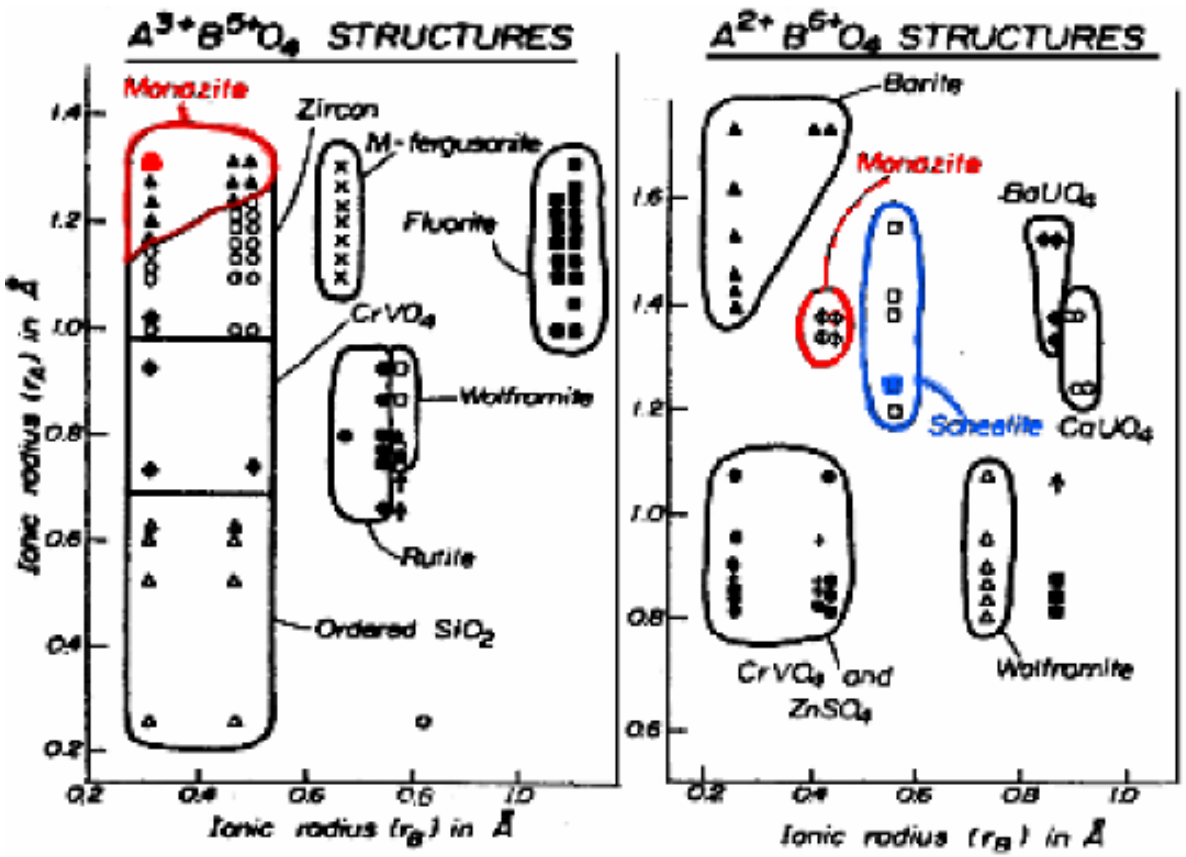
Monazite – $LaPO_4$



Monoclinic
mp 2072 °C
Hardness 5 GPa

Scheelite – $CaWO_4$

Tetragonal
mp 1580°C
4.5 GPa



Mechanical Properties Unexplored

Possible Applications

- Oxidation resistant CMC fiber-matrix interface
- Impact resistant TPS
- TBCs
- Machinable refractories
- Rad waste host
- Phosphors, tags
- T-t NDE indicator
- High Temperature Tribilogical Applications
- High Temperature Seals

Deformation Mechanisms

Objectives and Accomplishments for ABO_4 Oxides

Modeling and improvement of HT structural ceramics requires knowledge of their deformation mechanisms

Objectives

- **Measure mechanical properties & identify deformation mechanisms at σ, T**
- **Generalize mechanism models for simple materials to complex, low-symmetry materials**
- **Identify new materials, material combinations, textures, etc….**

Accomplishments (Monazite and Scheelite)

- **Fiber push-out – room and high temperature**
- **Single crystal and polycrystal indentation – LN_2 to 1000°C**
- **Optical, SEM, extensive TEM characterization**
- **Modeling using FEA and ERSS model, Mathematica programs for twinning prediction - extension to other complex oxides**

Far broader predictions possible via 1st principle routes