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Title: LANL Materials Capability Overview

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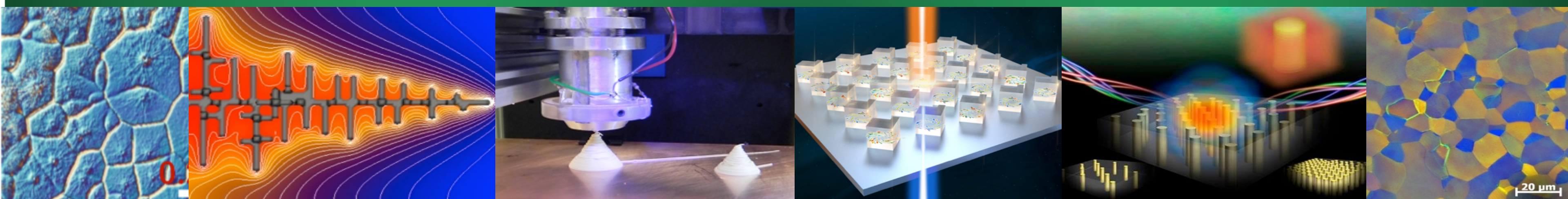
LANL Materials Capability Overview



Los Alamos NATIONAL LABORATORY EST. 1943

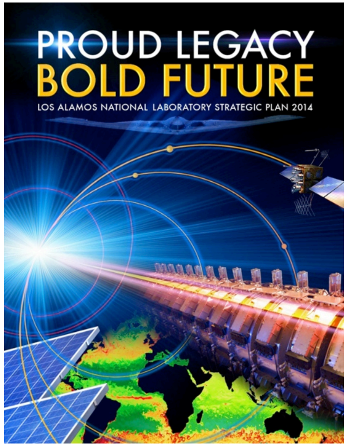
Ellen Cerreta, Division Leader

Materials Science & Technology

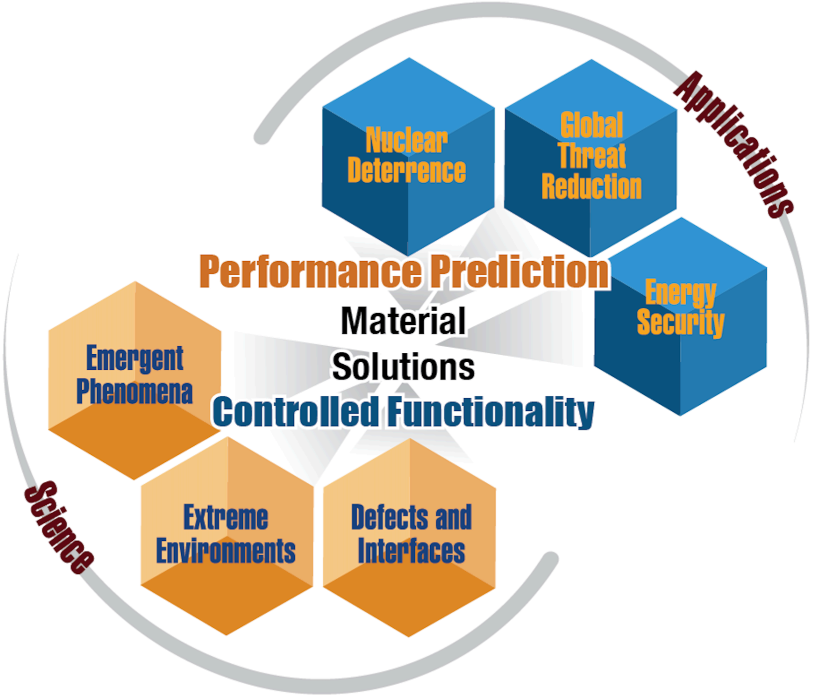
December 10, 2019

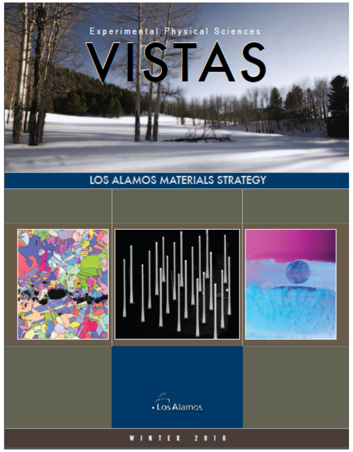
NNSA National Nuclear Security Administration

Our Vision Is to Develop Materials with Controlled Functionality and Predictable Performance



Solving the nation's toughest science and engineering challenges





Providing Materials Solutions to Address Mission Needs

Nuclear Deterrence – develop highly reliable, predictive tools to answer questions about performance in a changing stockpile due to aging, manufacturing, and material replacement.

Energy Security – includes materials for nuclear reactors, waste treatment, energy production, conversion and storage, transportation fuels and energy efficiency.

Global Security – includes addressing threats from peer adversaries and emerging nuclear threats; from the earliest adversary planning through resilient event response; as well as providing technical capabilities and expertise in support of global efforts to understand and limit nuclear proliferation through strengthening international nuclear safeguards and security.

Our Strategy Links Leadership Areas through Science Themes to Achieve Overarching Goals

GOALS

Performance Prediction and Controlled Functionality

SCIENCE THEMES

Defects and Interfaces

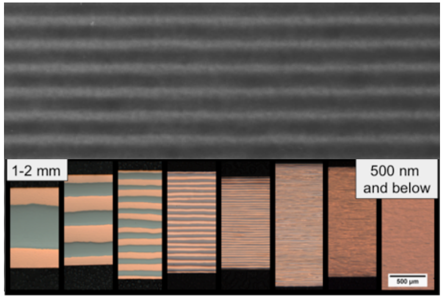
Extreme Environments

Emergent Phenomena

AREAS OF LEADERSHIP

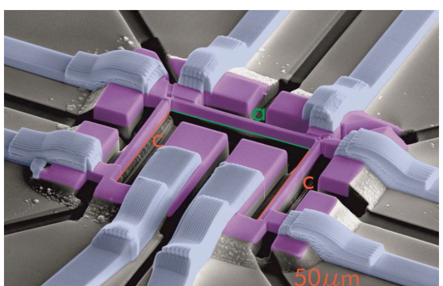
Complex Functional Materials	Material Resilience in Harsh Service Conditions	Manu-facturing Science	Actinides & Correlated Electron Materials	Integrated Nano-materials	Energetic Materials	Materials Dynamics

Three Science Themes Connect the AoLs



Defects and Interfaces – the mechanistic understanding and control of inhomogeneities, across all appropriate length and time scales, that govern materials functionality

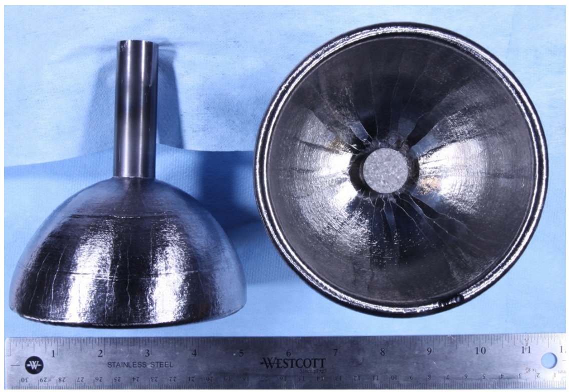
Extreme Environments – the underlying principles enabling the understanding of the interactions of materials with extreme conditions in order to create 1) environmentally tolerant properties and 2) the ability to exploit extreme environments to tune materials functionality

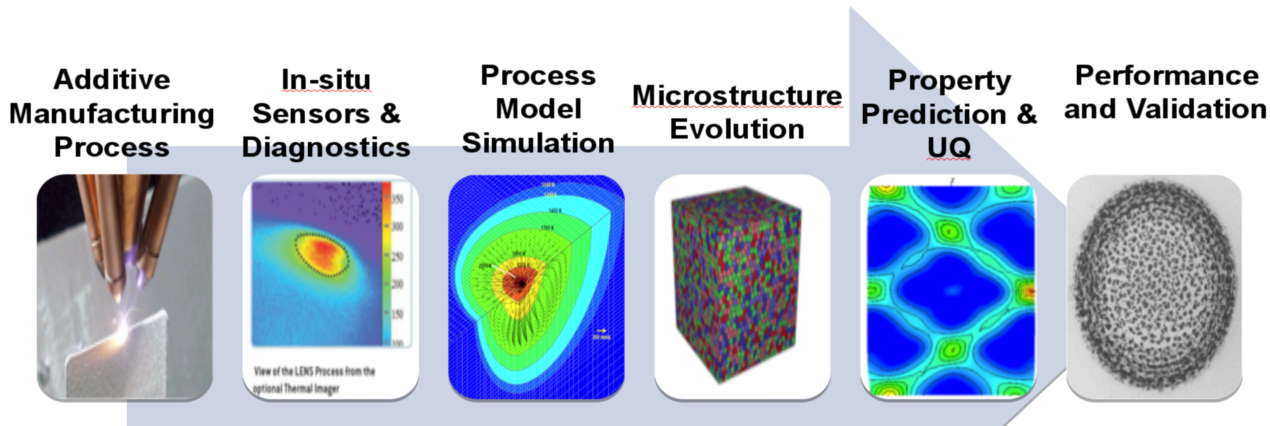


Emergent Phenomena – the science required to discover and understand complex and collective forms of matter that exhibit novel properties and respond in new ways to environmental conditions, enabling the creation of materials with innate functionality

Manufacturing Science is an Essential part of the LANL Materials for the Future Strategy

Manufacturing science can be defined as the application of fundamental science research and development activities in order to understand the critical steps in the manufacturing process for the purposes of control and optimization.



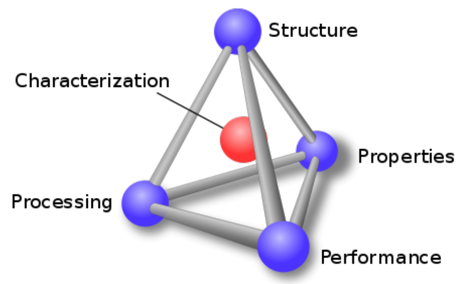


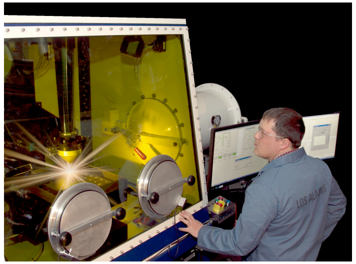
Some key areas where manufacturing science can help:

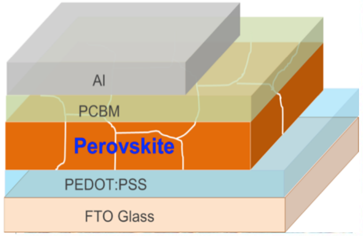
- Reduce experiments and increase understanding
- Qualification of new manufacturing methods such as additive manufacturing
- Scale up (size, quantity, equipment)
- Process control and rapid feedback
- Solve manufacturing problems on the floor

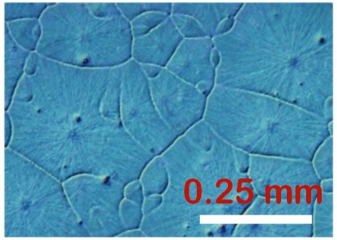
Manufacturing Science primarily supports LANL and NNSA Production Mission but also supports broader DOE programs

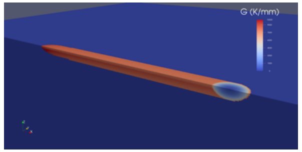
- Science basis for the processing-to-structure leg of the materials tetrahedron while recognizing its tie to properties and performance
- Development of the experimental and modeling tools to process materials with controlled functionality and predictable performance
- Develop novel synthesis or manufacturing techniques

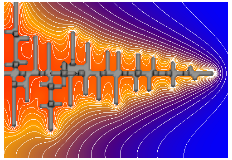








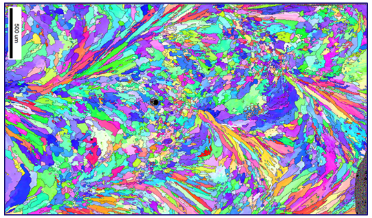




Process Modeling **Microstructure Modeling**

Our Mission requires that LANL is a Leader in Manufacturing Science

- **Longstanding capability in:**
  - discovery science and engineering
  - establishing design principles, synthesis pathways, and manufacturing processes
  - materials relevant to the U.S. nuclear deterrent, global threat reduction, and energy security challenges



- **Extensive expertise and capabilities:**
  - experimental, synthetic, characterization, and modeling expertise
  - conventional and additive manufacturing processes
  - metals, polymers, ceramics, foams, nanomaterials, and high explosives
  - classified, hazardous, and radiation environments
- **Unique span of capabilities from fundamental to prototyping to production:**
  - fundamental scientific studies of the manufacturing process
  - prototyping for energy and global security
  - production of parts for systems

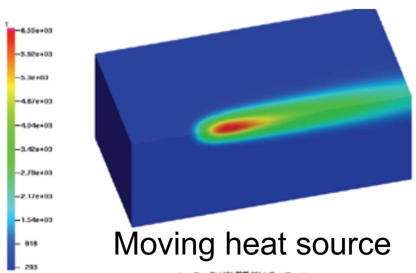
- **LANL's capabilities support production of weapons parts (pits and detonators).**

Materials Modeling and Computational Science are Critical to the Success of Manufacturing Science

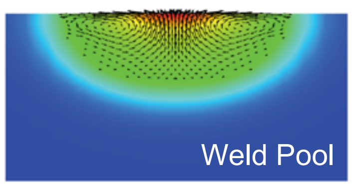
Process Modeling

TRUCHAS code

3D multiphysics microstructure-aware solidification capability



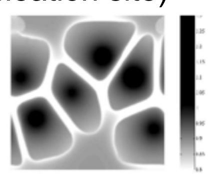
Moving heat source



Microstructure Modeling

Direct numerical simulation of grain growth

Initial grain distribution (Nucleation site)



Final grain shape and composition

Properties Modeling

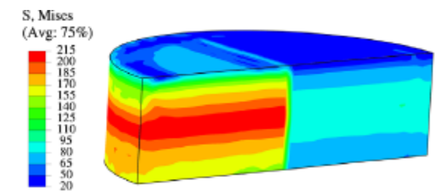
Polycrystal models to determine elastic/plastic/damage properties

Polycrystal and grain boundary properties

AM specific interface properties

Performance Modeling

Thermal - mechanical models to predict elastic/plastic/damage and failure processes



Mesoscale to macroscale prediction of performance

Liquid/solid phase change

Solid/solid phase transformation

The Capability Serves Deterrence Mission: Casting Unalloyed Pu

- Unalloyed plutonium is difficult to cast due to the 9% volume contraction during the beta to alpha transformation.
- **LANL produced unalloyed Pu via chill casting in the 1960s. We no longer have a chill casting capability and needed to determine a different method of achieving the same results.**
- **A combined experimental/modeling approach was used to develop the plutonium casting mold designs and process parameters and shorten the development time for casting.**

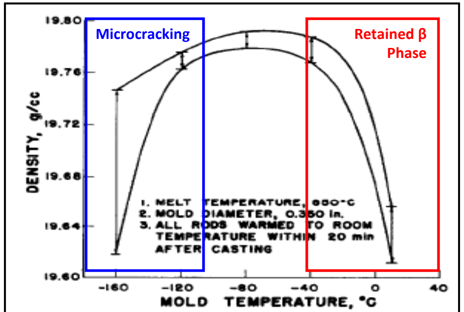
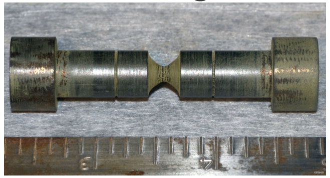


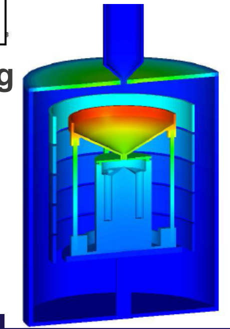
Fig. 3. Effect of mold temperature on ultimate densities of Pu rods.

1960s work using chill casting

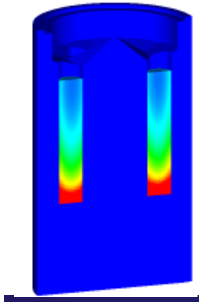


Full size δ Pu "D" notch tensile bar

Pu rod casting mold design for full size rods was developed using TRUCHAS to drive rapid cooling and edge to center transformation



Preheat Temperature



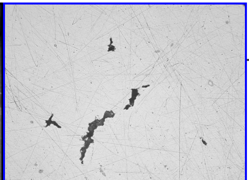
Fraction β→α Pu

The resulting rods had microcracks due to 2 problems:

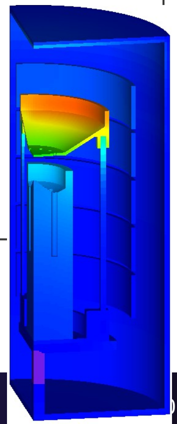
1) We used equilibrium property data for Pu. This data is insufficient to define phase transformations in Pu - kinetics, microstructure, and impurity composition are important.

2) The full size rods were too big to accommodate the transformation stresses using our available Pu casting equipment.

Ultimately, smaller rods were designed and successfully cast using updated property data and furnace constraints

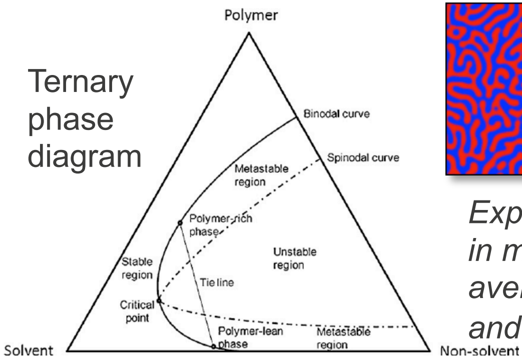


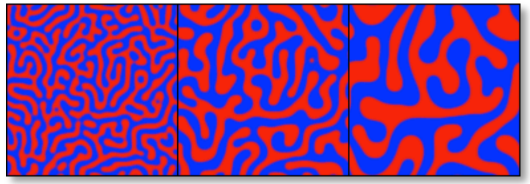
Pu micrograph with 100 μm crack



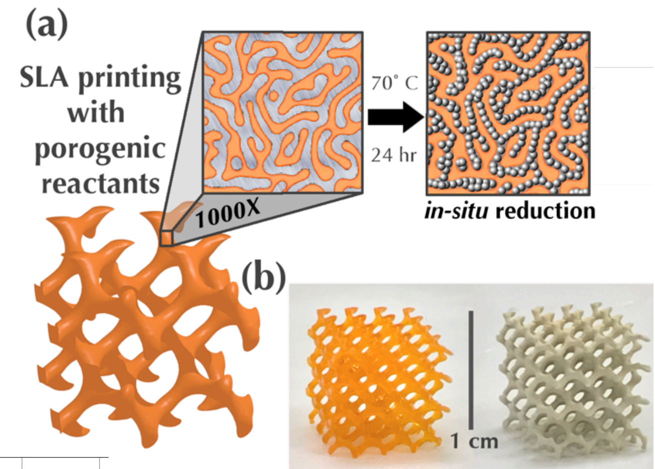
Advanced 3-D Printing Techniques Coupled with Complex Fluids Generate New Porous & Composite Materials

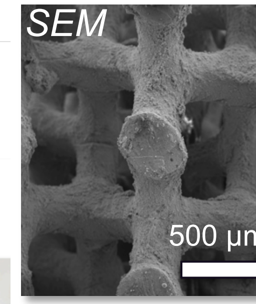
Ternary phase diagram





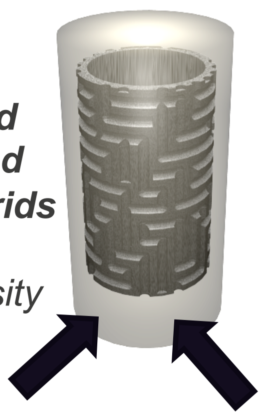
Exploiting complex phase behavior in multi-phase fluids opens new avenues to controlling chemistry and microstructure in materials.



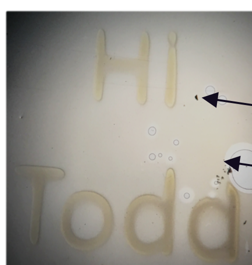


Metal-loaded polymer lattices

Engineered aerogel and metal hybrids

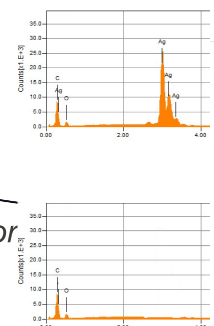


Low density matrix



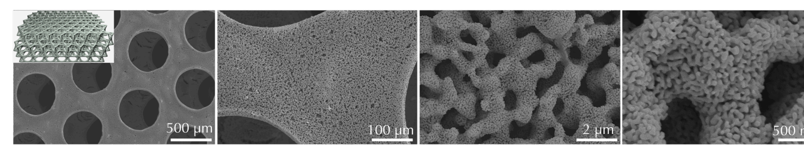
Ag-rich

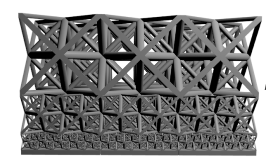
Ag-poor



Arbitrarily metalized regions within 3-D printed aerogels

Nested-Network Metallic Foams





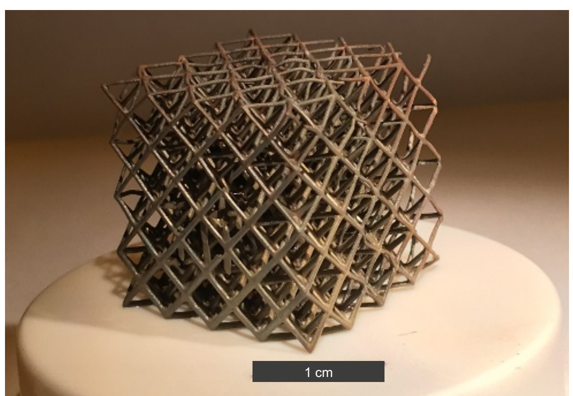
Graded-density metals and polymers

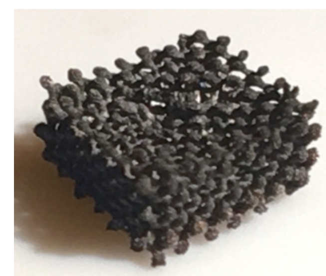
Similar Methodology Is Used for the Development of High Temperature Ceramics and Composites

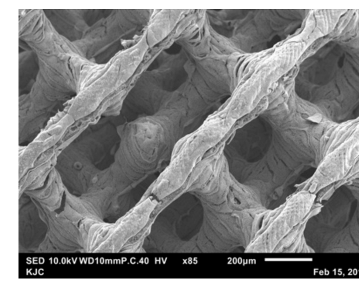
Various carbide materials are derived from 3-D printed "green parts" with a single heat treatment step

1400˚C

Conductive polymeric composites are printed directly using nanoparticle and/or ionic fillers







Non-traditional AM materials such as Iron may be derived directly from 3-D printed molecular precursors

In Summary

- Our materials strategy is dedicated to the development of materials with controlled functionality and performance that we can readily predict
- Our materials program is focused on understanding the deterministic relationship between processing and performance
- Our deterrence mission requires us to be leaders in Manufacturing Science – with an increased emphasis to consider advanced manufacturing processes and development of new materials
  - Reliant on advanced modeling and computational tool capabilities
- Our involvement in broader DOE programs allows us to exercise this capability to examine a wide range of performance requirements
  - For these customers it provides access to significant NNSA capability investment