



A Path Forward for Integrated Computational Materials Engineering in Support of Additive Manufacturing at NASA

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**JANNAF Additive Manufacturing for Propulsion Applications TIM
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Outline



- **NASA Missions**
- **Computational Materials**
- **ICME for Additive Manufacturing**
- **Concluding Remarks**



President Obama at KSC – April 15, 2010

“Early in the next decade, a set of crewed flights will test and prove the systems required for exploration beyond low Earth orbit. And by 2025, we expect new spacecraft designed for long journeys to allow us to begin the first-ever crewed missions beyond the Moon into deep space. So we’ll start -- we’ll start by sending astronauts to an asteroid for the first time in history. By the mid-2030s, I believe we can send humans to orbit Mars and return them safely to Earth. And a landing on Mars will follow.”

• NASA Authorization Act of 2010 & 2012 Appropriations

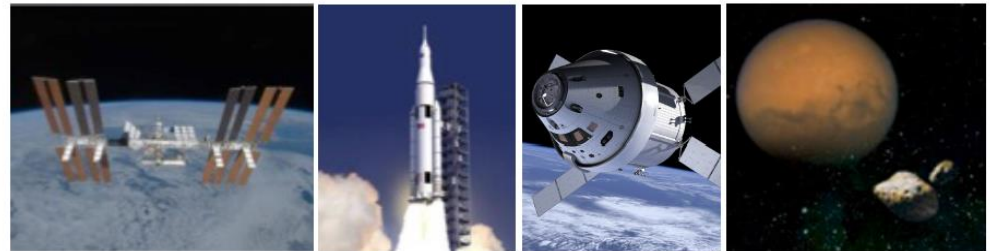
- Bipartisan support for human exploration beyond low Earth orbit, signed by President Barak Obama

• The law authorizes:

- Extension of the International Space Station until at least 2020
- Support for a commercial space transportation industry
- Development of a Multi-purpose Crew Vehicle and heavy lift launch capabilities
- A “flexible path” approach to space exploration opening up vast opportunities including near-Earth asteroids (NEA), moon, and Mars
- New space technology investments to increase the capabilities beyond low Earth orbit

• FY13 President’s Budget Request

- Asteroid by 2025, Mars orbit by mid-2030s



* Adapted from J. Crusan, “NASA’s Human Space Exploration Capability Driven Framework,” Briefing to the National Research Council Committee on Human Spaceflight, 2013.

The Future of Human Space Exploration*



- One-way transit times to destinations



* Adapted from J. Crusan, "NASA's Human Space Exploration Capability Driven Framework," Briefing to the National Research Council Committee on Human Spaceflight, 2013.

A New Paradigm is Needed for the Mission to Mars



250 miles
International
Space Station

Today's strategy for LEO does not work for tomorrow's deep space missions

Today, we rely on the 4 R's: resupply; repair by replacement; redundant hardware; retreat to earth

For Mars and beyond: a new paradigm is needed – can basic research help? History shows it has and will.



Martian Sunset
33,900,000 miles

Elements Required by Potential Destination*



Phase	Capability	Potential Required Element	For Potential Destinations			
			L1/L2	Asteroid	Mars Orbit / Moons	Mars Surface
Getting There	BEO Access	Space Launch System (SLS)	X	X	X	X
	Crew	Orion	X	X	X	X
	High Thrust/Near Earth	Cryo Propulsion Stage (CPS)	X	X	Option	Option
	Low Thrust/Near Earth	Solar Electric Propulsion (SEP)	Option	Option	Option	Option
	High Thrust/Beyond LEO	Nuclear Thermal Propulsion (NTP)	Option	Option	Option	Option
	Low Thrust/Beyond LEO	Nuclear Electric Propulsion (NEP)	Option	Option	Option	Option
	Habitation	Habitat	Option	X	X	X
	Descent	EDL / Landers				X
Working There	Habitation	Habitat				X
	Micro-g Sortie and Surface Mobility	Robotics and Mobility		X	Option	X
	In Situ Resource Utilization	In-Situ Resource Utilization (ISRU)				X
	Surface Power	Fission Surface Power System				X
	EVA (nominal)	EVA Suits	X	X	X	X
Coming Home	Ascent	Ascent Vehicle				X
	Crew Return	Orion	X	X	X	X

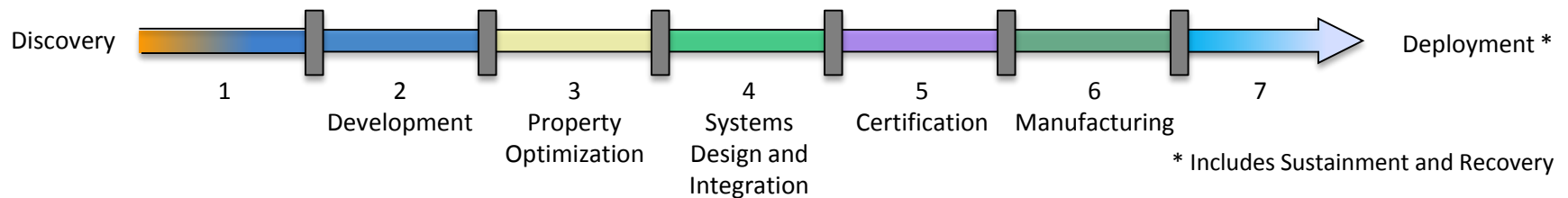
Note:
X – Required Elements/Capabilities for these potential destinations
Option – Element/Capability may be needed or multiple options could exist to enable missions for that specific potential destination or could be for verification for future needs.

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* Adapted from J. Crusan, "NASA's Human Space Exploration Capability Driven Framework," Briefing to the National Research Council Committee on Human Spaceflight, 2013.

Materials State of the Art

- Materials development relies on scientific intuition and trial and error experimentation.
- Numerous repetitive experiment and characterization loops.
- Multiple discreet steps performed by different teams at different facilities.
- Lengthy and costly design and insertion cycles.



Materials Development Continuum ¹



The Lab of the 20th Century

- **Lots of “data”**
- **Little understanding**
- **Supported engineering by heuristics**
- **Primarily legacy metallic alloys and polymeric composites**

¹ Materials Genome Initiative Strategic Plan, https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

National Materials Genome Initiative



Announced in Jun 2011 by President Obama¹:

Vision: Advanced materials are essential to economic security and human well-being and have applications in multiple industries, including those aimed at addressing challenges in clean energy, national security, and human welfare. To meet these challenges, the Materials Genome Initiative will enable discovery, development, manufacturing, and deployment of advanced materials at least twice as fast as possible today, at a fraction of the cost.

Strategic Goals:

- (1) Leading a culture shift in materials-science research to encourage and facilitate an integrated team approach;
- (2) Integrating experiment, computation, and theory and equipping the materials community with advanced tools and techniques;
- (3) Making digital data accessible; and
- (4) Creating a world-class materials science and engineering workforce that is trained for careers in academia or industry

¹ Materials Genome Initiative Strategic Plan,
https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

National Materials Genome Initiative



Integrated Computational Material Engineering (ICME) is critical for development and certification of new materials and processing techniques.

It's not just computational modeling...



Materials Genome Initiative Overview ¹

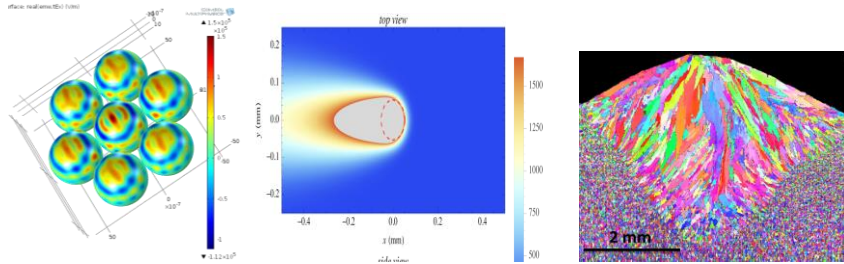
- Experimentation: Strategically defined experiments used to evaluate variables and validate computational models.
- Characterization: Detailed examination of all aspects of material properties (microscopy, NDE, surface finish, mechanical properties, etc) to provide verification data for computational models
- Modeling: Fundamental physical understanding and computational tools/models used to predict behavior.

¹ Materials Genome Initiative for Global Competitiveness, http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

ICME for Additive Manufacturing Multi-scale and Multi-physics Modeling



Processing Modeling

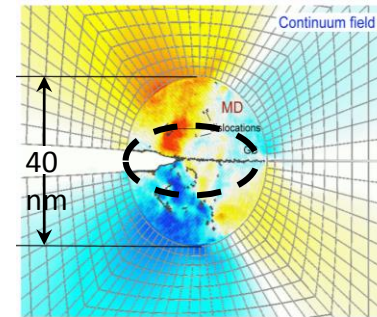


Melt Pool Modeling

Microstructure Evolution

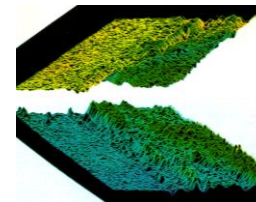
Thermal Modeling

Performance Modeling



Molecular Dynamics

Microstructure Models

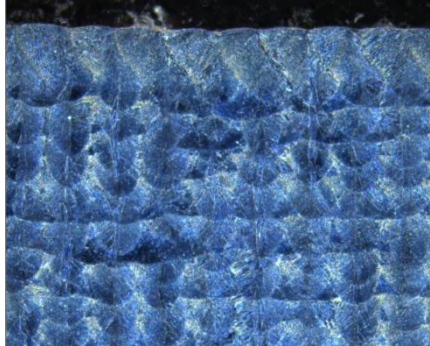


Damage Science

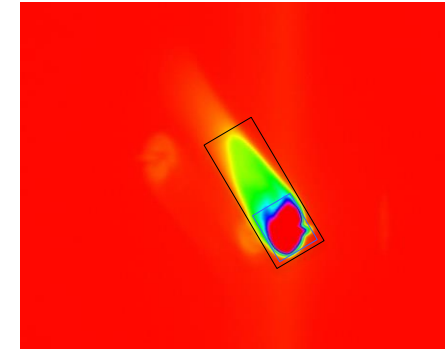


Structure

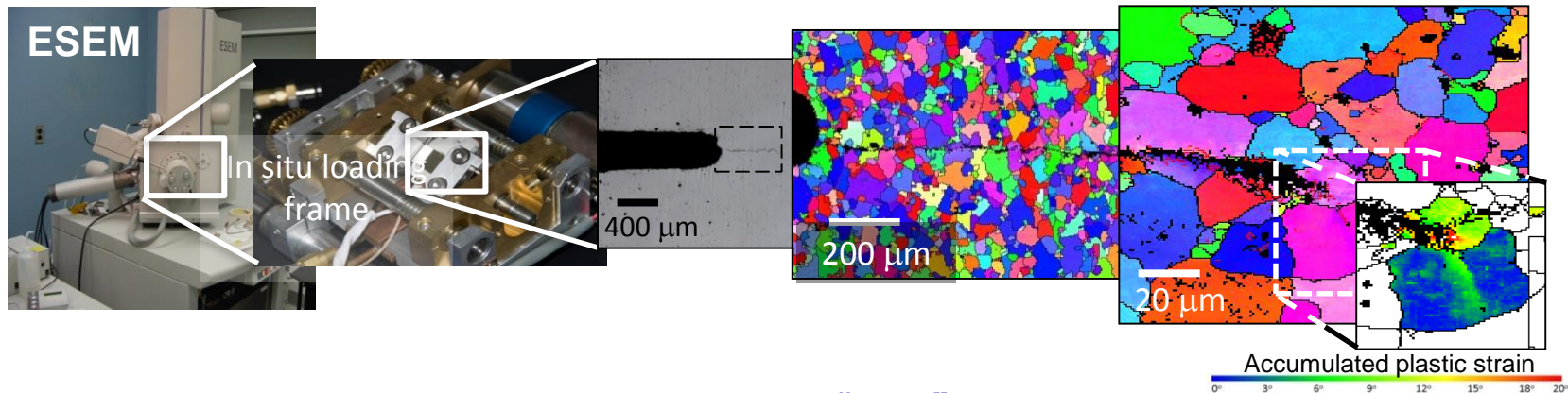
ICME for Additive Manufacturing Experimentation and Characterization



Microstructural Characterization



In-Situ Monitoring of AM



- More thoughtful acquisition of “data”
- More understanding of what the “data” means
- More collaboration with NDE and material developers
- Support “physics-based” computational methods

ICME for Additive Manufacturing



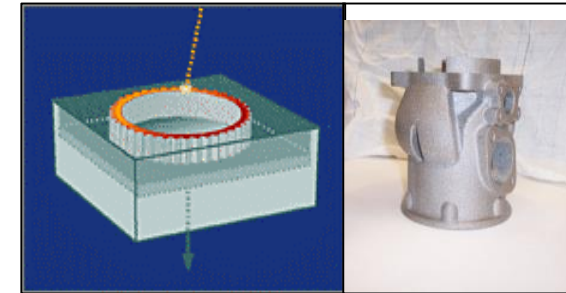
Goal: Successful build of certified components on first try

Near-term impacts:

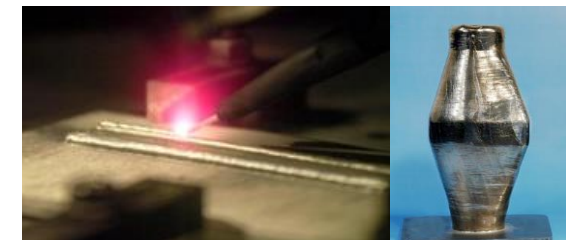
- Optimize material build parameters with reduced time and cost
- Increase understanding of build properties & reliability of builds
- Decrease time to adoption of process for critical hardware
- Provide data for certification documentation and process qualification
- Assist feedback control using in-situ monitoring
- **DARPA Open Manufacturing systems level study has determined current computational approaches will yield 40% reduction in time and 20% reduction in cost**

Far-term opportunities:

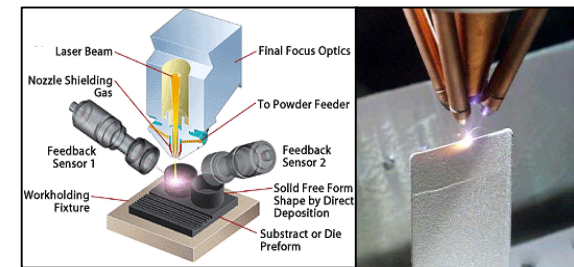
- Understand effect of non-conforming process monitoring data (e.g. hot or cold spots)
- Modify CAD using predicted distortions (from residual stresses)
- Design tailored materials for improved performance



Laser Sintering/E-beam Melting

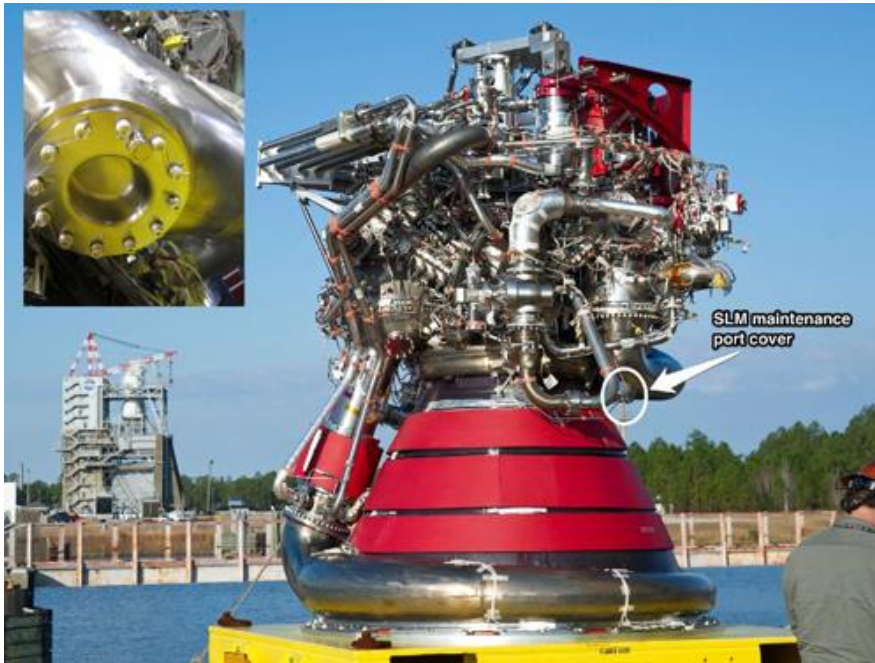


Electron Beam Freeform Fabrication

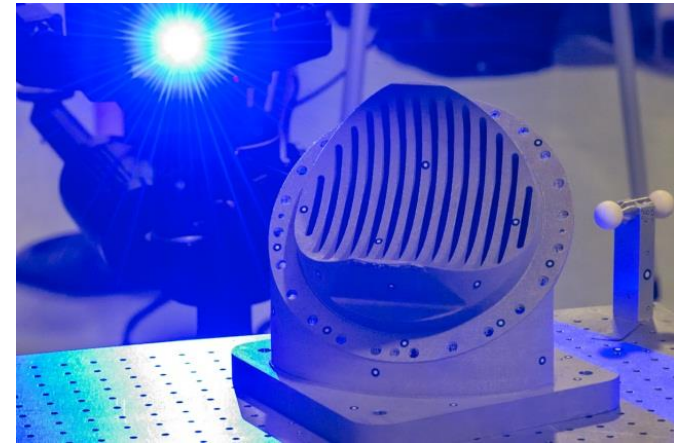


Laser Net Shaping

Additive Manufacturing in SLS



RS-25 Engine prior to testing
at Stennis Space Center



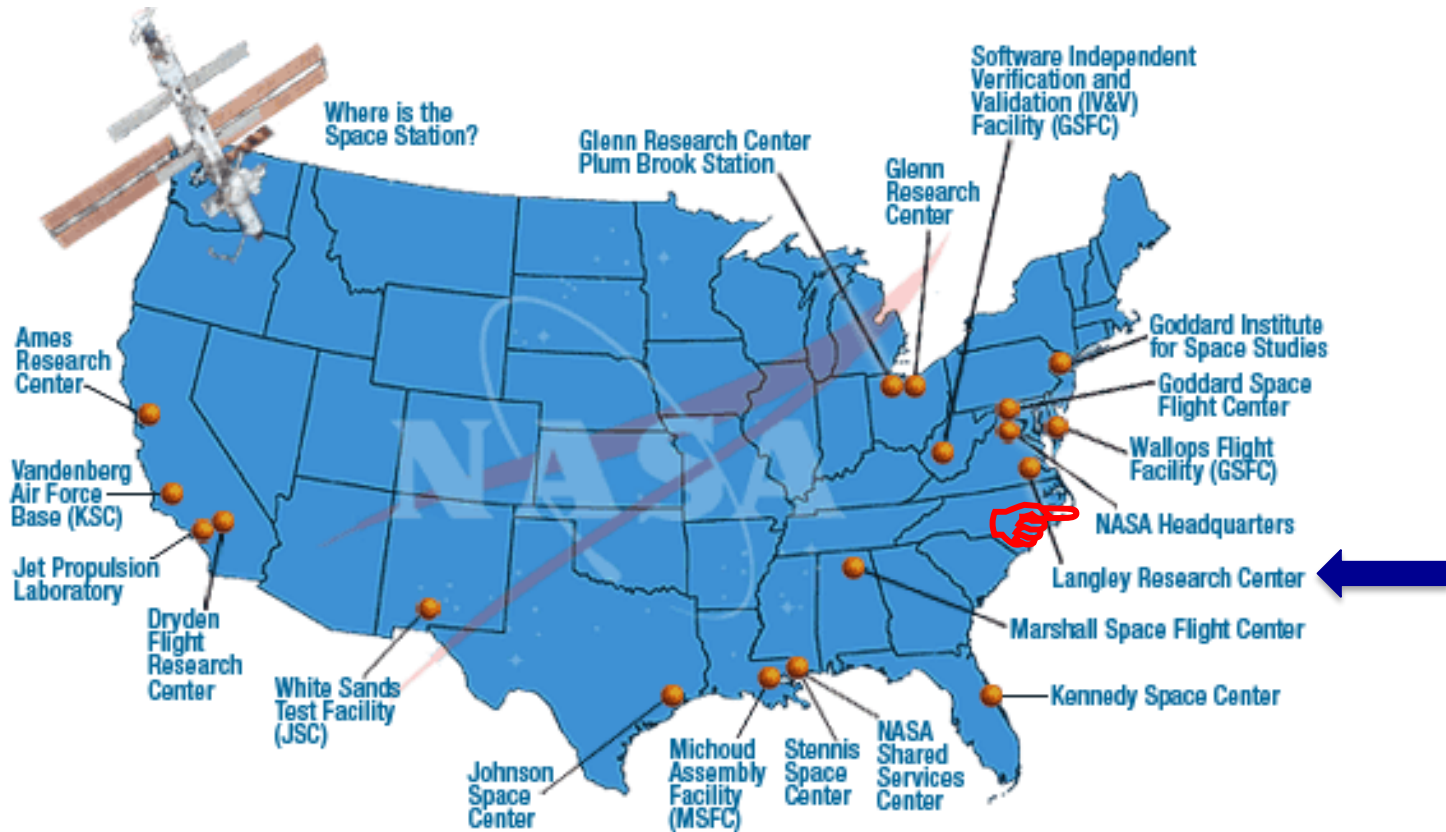
Pogo Z-Baffle made from
Selective Laser Melting (SLM)

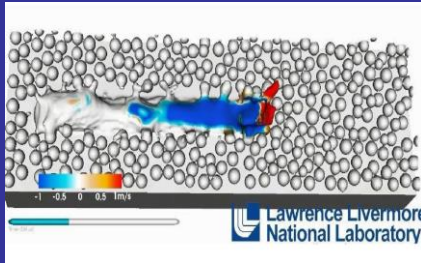
What can MGI do for SLS

- Improve Process Certainty
 - Design / Tailor Process
- Improve Part Certainty
 - Meet material specifications
 - Certify components

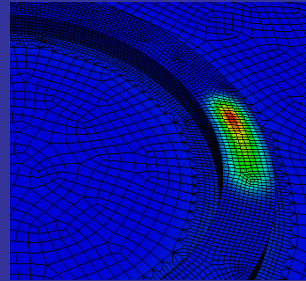


NASA Centers





Simulation of Laser-Powder Bed Interactions



Prediction of Local Heat Distribution

Simulate Fundamental Physics Governing Processing

- Simulate physical processes including laser beam absorption in powder bed, heat transfer via conduction and radiation, and fluid flow at the melt pool, particle flow
- Simulate residual stress, distortion, microstructural evolution and precipitate growth

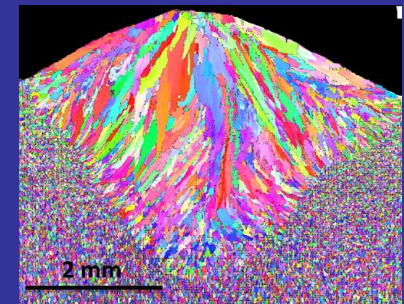
Develop Physically Correct Models Needed to Support Certification of AM Feed Stock and Manufacturing Process

Characterize Material Evolution using Experimental Methods

- Employ heavily-instrumented SLM machine
- Produce coupon-size specimens using well-controlled parameters
- Understand details of the relationship between processing parameters and resulting microstructure



Selective Laser Melting



Grain Structure from Additive Process

In-Situ Monitoring of Additive Manufacturing



Approach

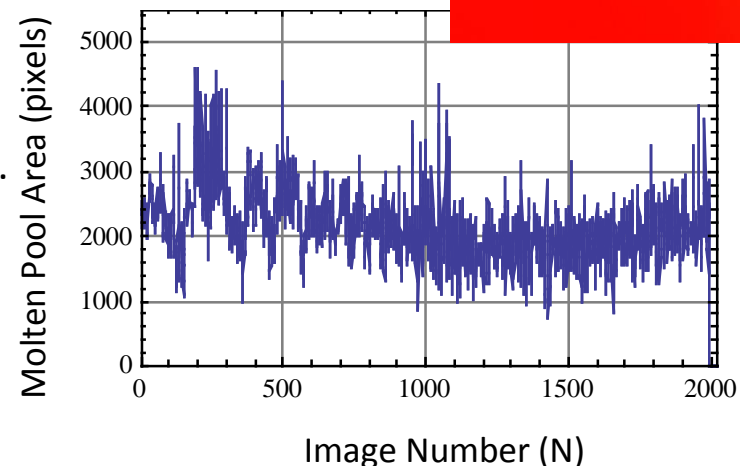
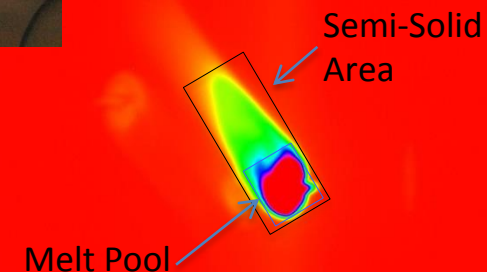
Use spatial and radiometric calibrated infrared thermography to remotely acquire temperature images and apply advanced image processing techniques to determine deposition parameters such as molten pool size and semi-solid area in real time using tracking algorithm.

Results

- Imaged and measured deposition parameters such as melt pool area and semi-solid regions.
- Able to track melt pool and semi-solid area independent of orientation.
- Able to provide much greater resolution than in QM melt pool system (1,000's pixels vs. 9 pixels).



Real Time Tracking

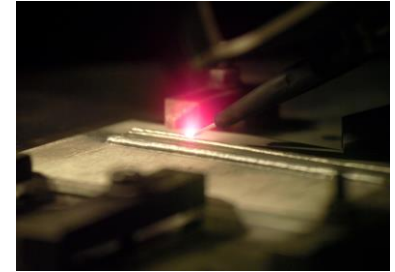


• Description of the FE Model

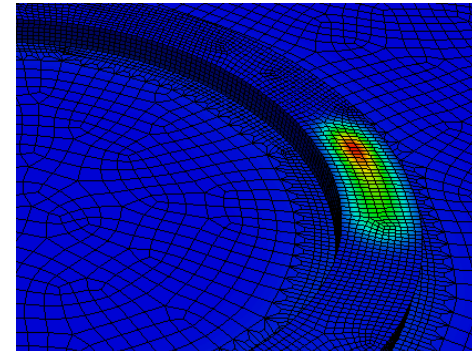
- Transient heat diffusion with phase change
- Set up model using final part geometry
- Activate elements for the added powder per layer
- Heat input model defines the distribution of volumetric heat source (units are $\text{J}/\text{m}^3\text{-sec}$)

• Details

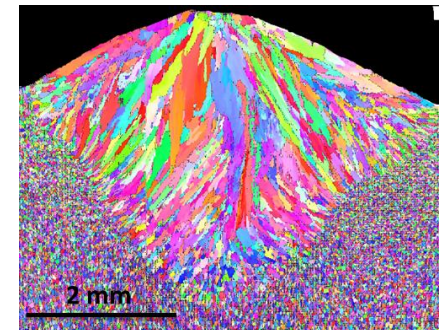
- Currently only heat diffusion is modeled in order to predict the thermal history for the entire part (thermal cycling will occur in the layers)
- Convection and radiation boundary conditions included
- All of the “action” takes place in the melt pool, requiring a very fine mesh to capture the steep gradients. This leads to high computational costs when modeling numerous layers.
- Convection within the melt pool is captured by artificially increasing the conductivity of the melted material (factor of 2 [Yaghi 2012])
- The effect of different heat input models is insignificant away from the melt pool zone



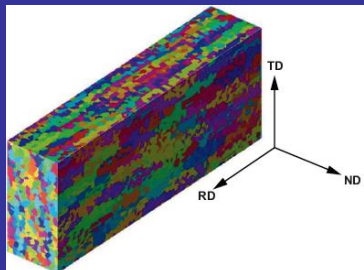
EBF3 (also SLM)



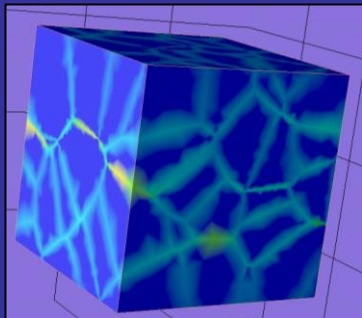
Local Heat Distribution



EBSD of SS316 Single Layer Build



Replication of As-Manufactured Material Microstructures



Predictions of Crack Initiation and Growth

Simulate Operative Physical Processes at Relevant Length Scales

- Develop simulations that address operative physical mechanisms
- Simulate as-manufactured materials to understand role of microstructure on lifecycle performance
- Incorporate material informatics to parse the vast parameter space

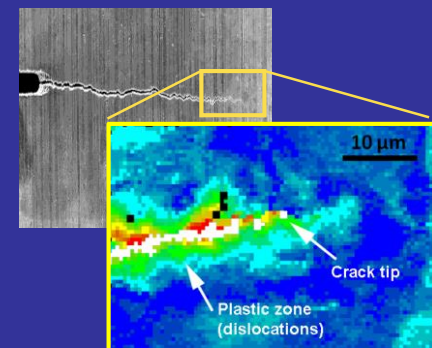
Develop Microstructure-Sensitive Fatigue Crack Growth Model Needed to Support Certification of AM Components

Characterize Material Response using In-Situ Experimentation

- High resolution X-ray CT to determine void/phase content of as-manufactured materials
- In-situ testing for determination of operative mechanisms and simulation validation
- High resolution strain and damage maps to understand microstructural influences on damage

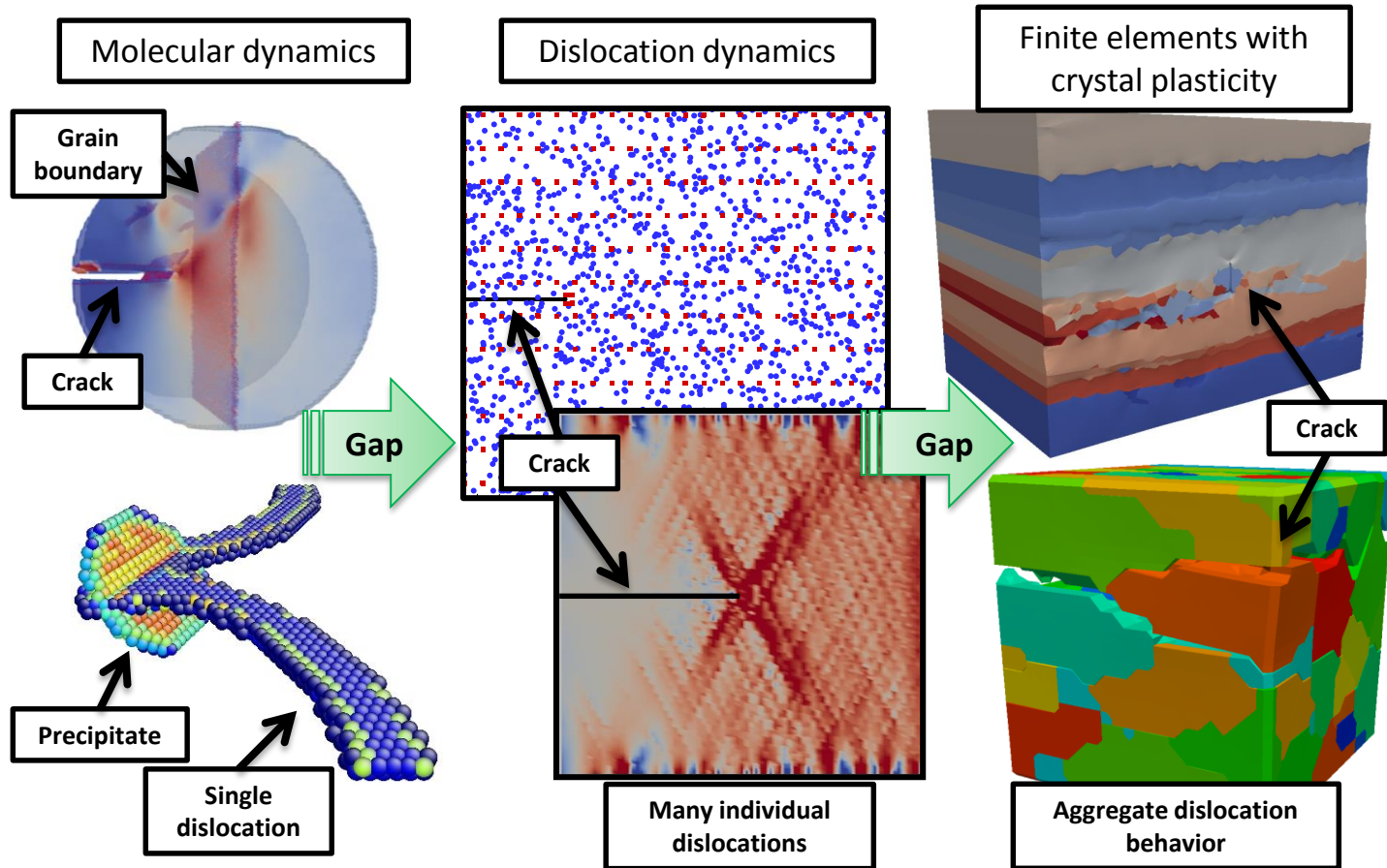


Mechanical Testing Inside a SEM



Characterization of Damage Evolution

ICME for Material Performance



ICME for Material Performance

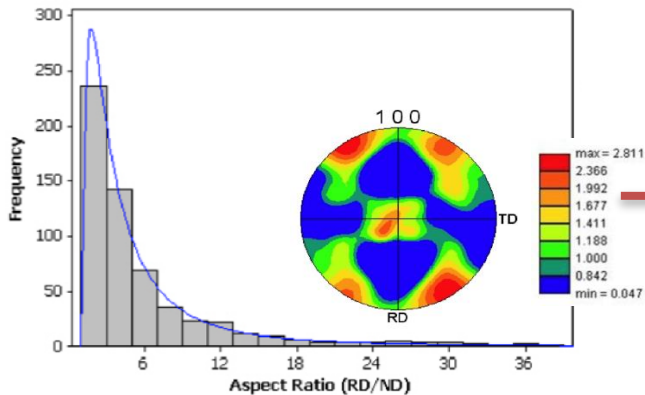
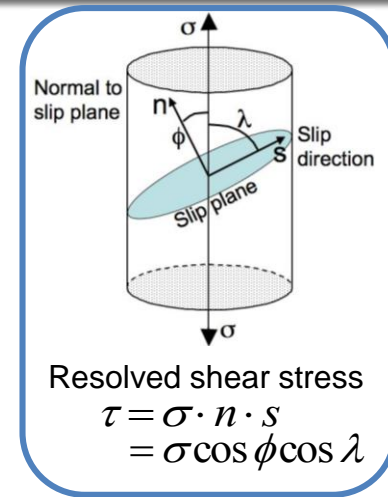
Constitutive equation for slip
on slip system α

$$\dot{\tau}^{\alpha} \geq \tau_c^{\alpha} = \sum_{\beta=1}^n h_{\alpha\beta} \dot{\gamma}^{\beta}$$

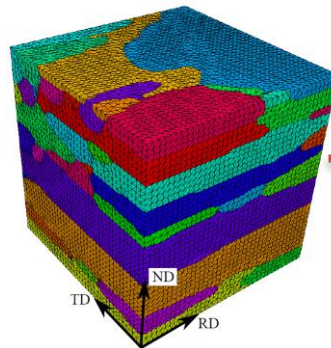
where

$h_{\alpha\beta}$ \equiv hardening modulus

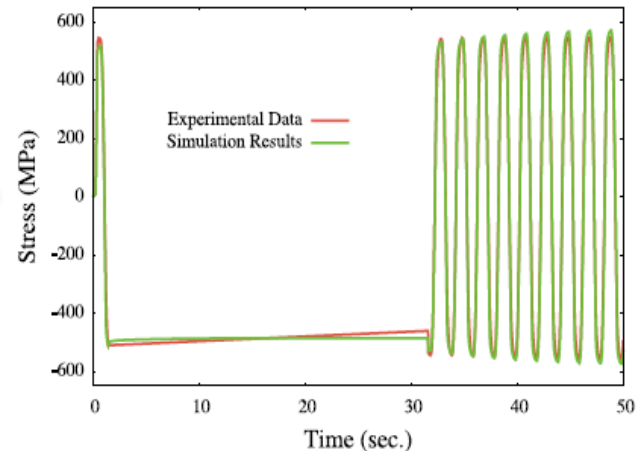
$\dot{\gamma}^{\beta}$ \equiv slip on slip system β



Characterize Microstructure Morphology



Generate a Digital Polycrystal

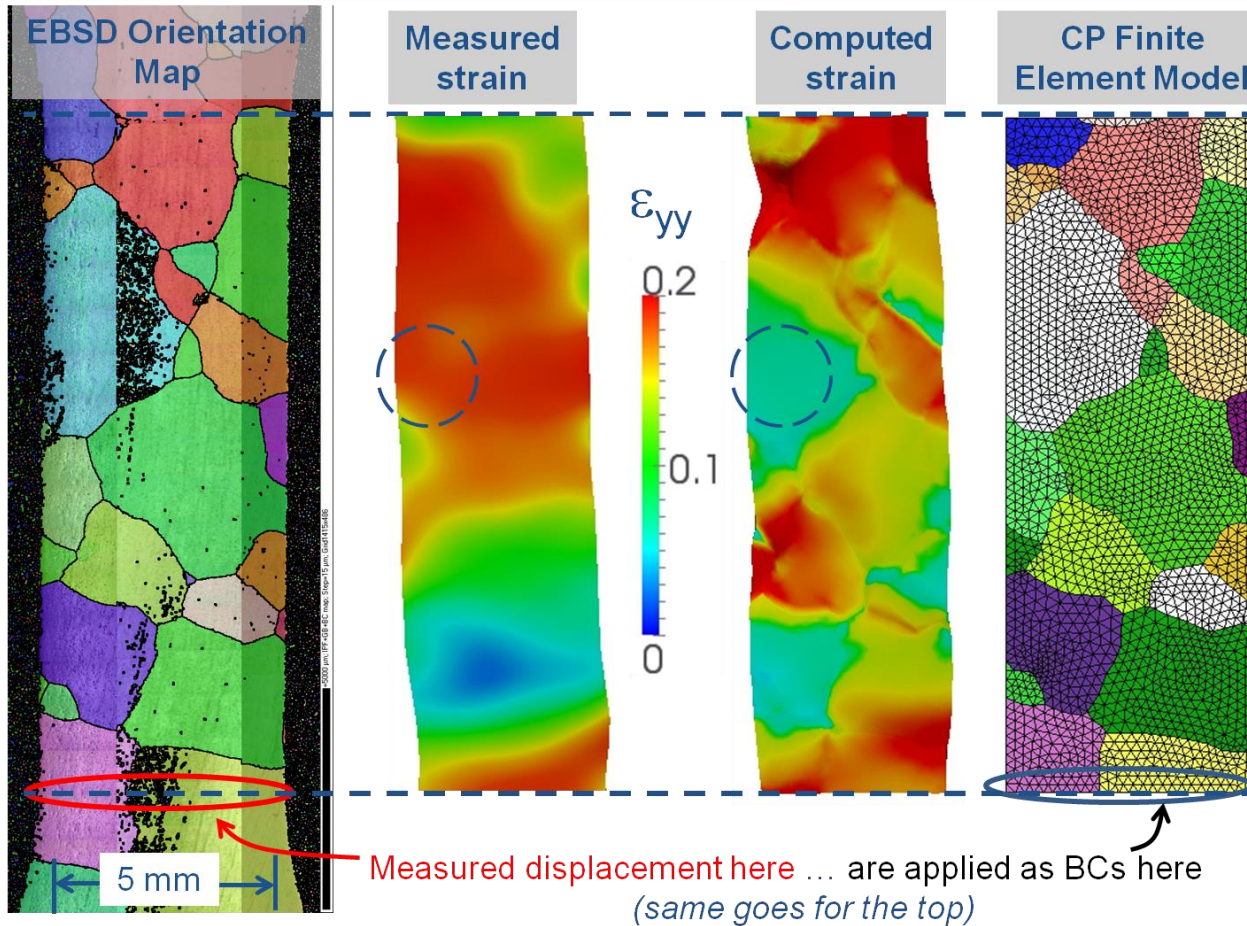


Parameter Calibration

Parameters determined from response of polycrystals and assumed valid on all slip systems

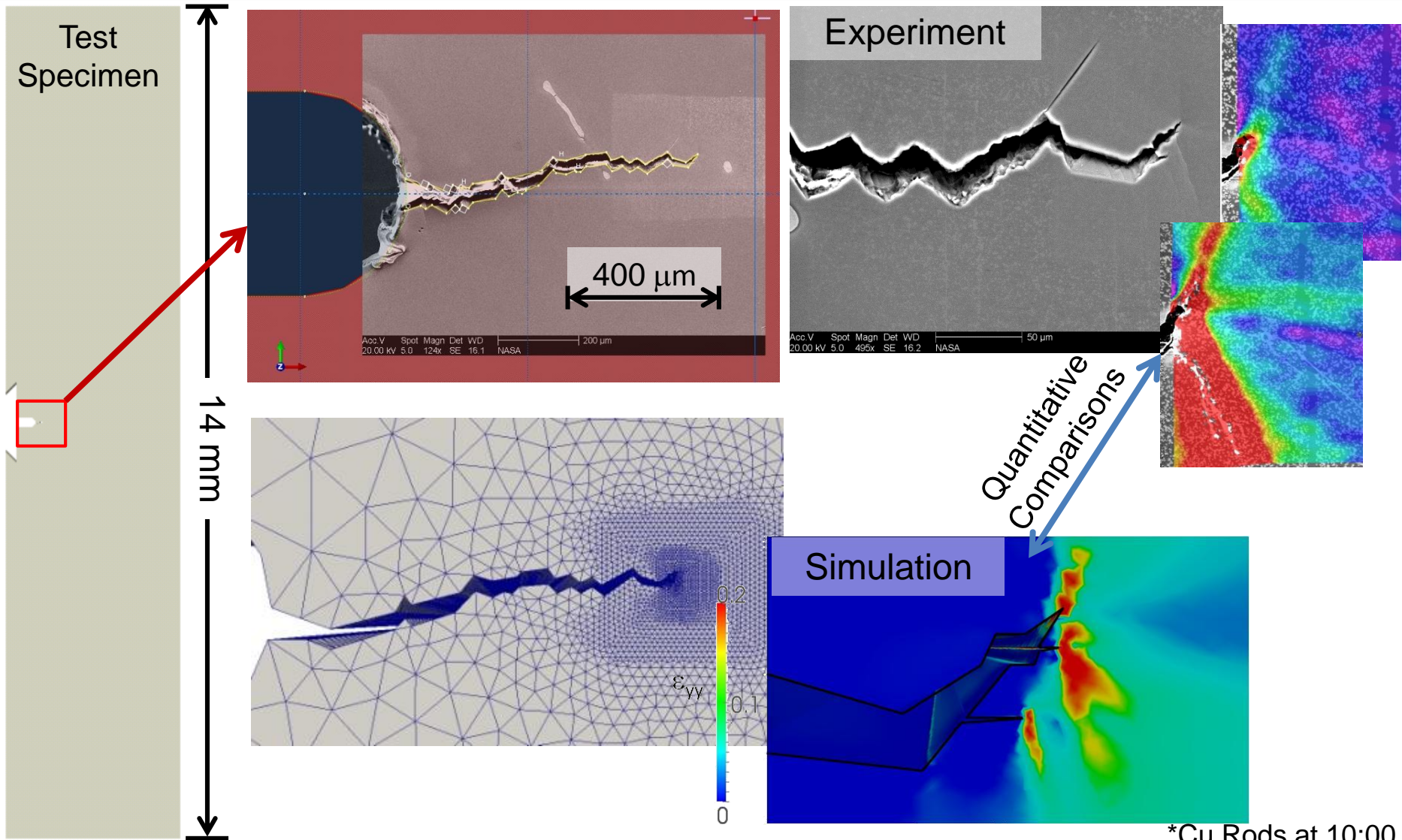
*Mantous and Maniatty, IJNME, 60, 2004, p. 2313.

ICME for Material Performance



Simple ~2D configuration with replicated grains

ICME for Material Performance



Quantitative Comparisons

*Cu Rods at 10:00

Concluding Remarks



- **New materials and processing capabilities are enabling to future NASA missions**
- **The National Materials Genome Initiative (MGI) offers a framework for Integrated Computational Materials Engineering (ICME) approaches to decrease the current cost and time for materials and processing development**
- **Successful ICME requires develop and integration of computational models, experimental and characterization techniques**
- **Foundational research is currently being conducted at NASA to address these technical challenges**