The Materials Genome Initiative and Additively Manufactured Metals: New Computational Tools and the Central Role of Materials Data

Peter Voorhees, Greg Olson, Begum Gulsoy | *Northwestern University*
Juan De Pablo | *University of Chicago*

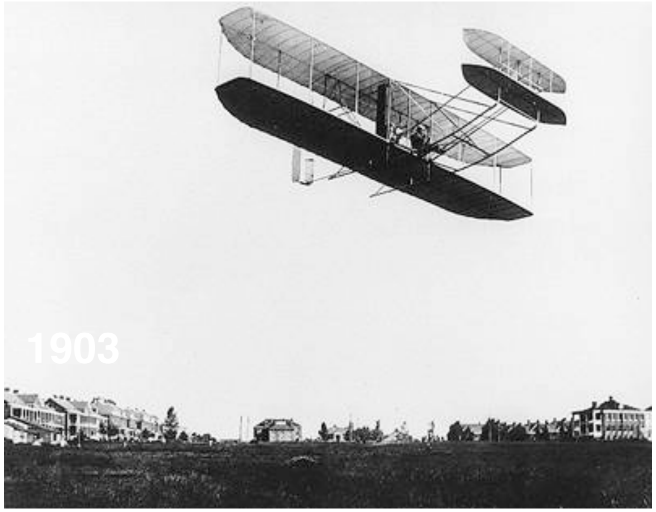
Alexander Chadwick, Northwestern University

NIST

Office of Naval Research Science & Technology

CHIMaD

Challenge of Materials Development

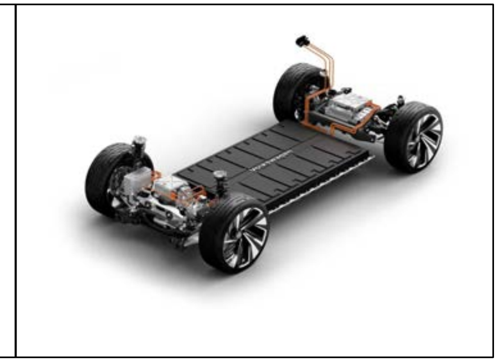


"$Al_{92}Cu_{8}$" → "Al 319"

$Al_{88.08}Si_{7.43}Cu_{3.33}Mg_{0.22}Fe_{0.38}Mn_{0.24}Zn_{0.13}Ti_{0.12}Ni_{0.01}Cr_{0.03}Sr_{0.03}$

CHiMaD

Challenge of Materials Development



Newer materials also follow a 20-year development cycle

1970	**1991**	**2020**
Exxon	**SONY**	

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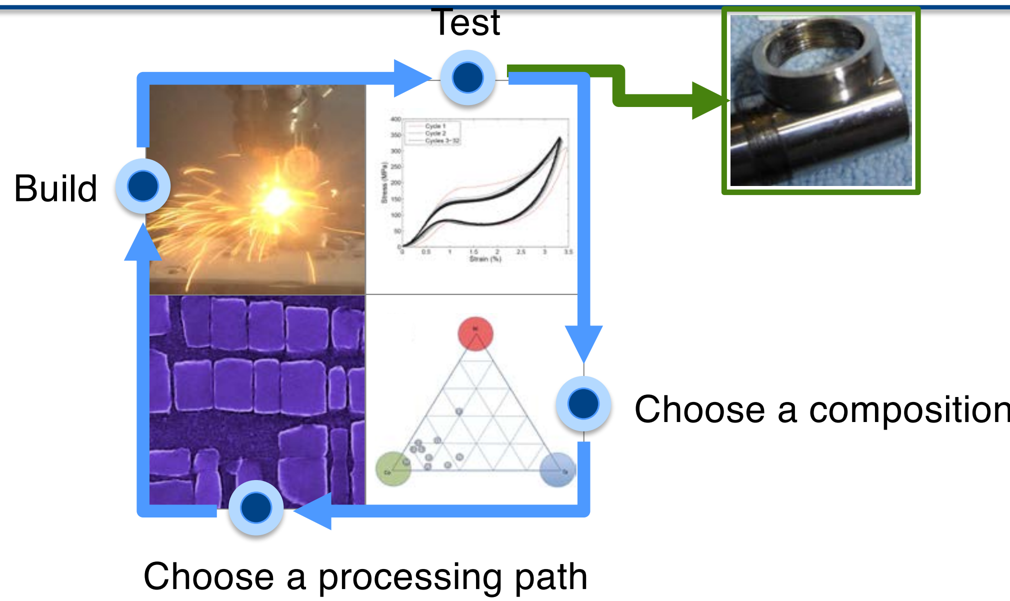
Conventional Approach



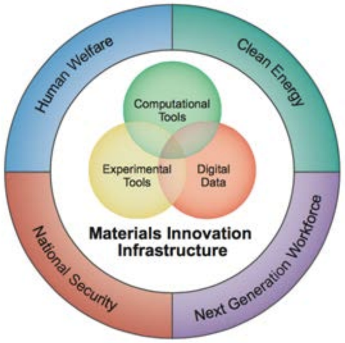
High-cost = Barrier to the introduction of new materials

Recertification requirement = Prevents even minor changes

Materials Genome Initative

"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."
MGI Strategic Plan 2014

- Developing a Materials Innovation Infrastructure
  - Integrating experiments, computations, data, and machine learning
  - Open-access/Open-source
- Achieving National Goals with Advanced Materials
  - Develop the *infrastructure* to design new materials
- Equipping Next Generation Materials Workforce
- Engaging all stakeholders



Result: A new design paradigm wherein
the material and the device are designed *simultaneously*

CHIMaD

Integration of computational DATA & tools to reduce time and/or cost

Industry / Public Domain

SUCCESS STORIES

Image from: https://www.macworld.co.uk/review/apple-watch/original-apple-watch-review-3544044/

Apple New Alloys

New alloys developed for Apple Watch:
Stainless steel - Aluminum - Gold

Materials Innovation Case Study:

Corning's Gorilla® Glass 3 for Consumer Electronics

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

https://www.CorningGorillaGlass.com

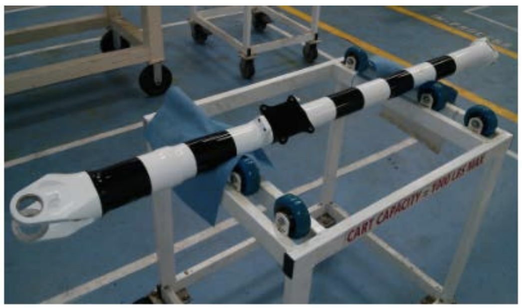
- Version 3 – 2013 - Clean sheet to production in **22 months**
- At the end of 2015 Gorilla Glass was used in 4.5 Billion+ devices
- Success is a result of **verified computational tools** , **experience** with previous versions and fundamental research
- No need for certification

https://www.nist.gov/sites/default/files/documents/2018/06/26/materials_innovation_case_study_gorilla_glass_3_020816.pdf

Materials Innovation Case Study:

QuesTek's Ferrium® M54® Steel For Hook Shank Application

National Institute of Standards and Technology
U.S. Department of Commerce



- Clean sheet to production in **7 years**
  - 3 years for formal qualification
- Use of computational tools to predict the variability in properties introduced by the manufacturing process
- Greatly reduced the time required for qualification: very few heats
- Success is a result of **accurate databases** for Fe-based materials and **verified computational tools**

https://www.nist.gov/sites/default/files/documents/2018/06/26/materials_innovation_case_study_questek_090616.pdf

SpaceX Superalloys

New superalloy developed for Raptor Rocket Engine

alicia hamblin @leechy3 · Jun 17, 2018
Replying to @elonmusk and 2 others
I heard new alloys...I'm interested! What types of alloys are you currently using on the rocket?

Elon Musk @elonmusk

SX 300 & soon SX 500. Kind of a modern version of Inconel superalloys. High strength at temperature, extreme oxidation resistance. Needed for ~800 atmosphere, hot, oxygen-rich turbopump on Raptor rocket engine.

615 11:25 AM - Jun 17, 2018

Elon Musk @elonmusk

Follow

Replying to @Robotbeat @Jon128123 and 7 others

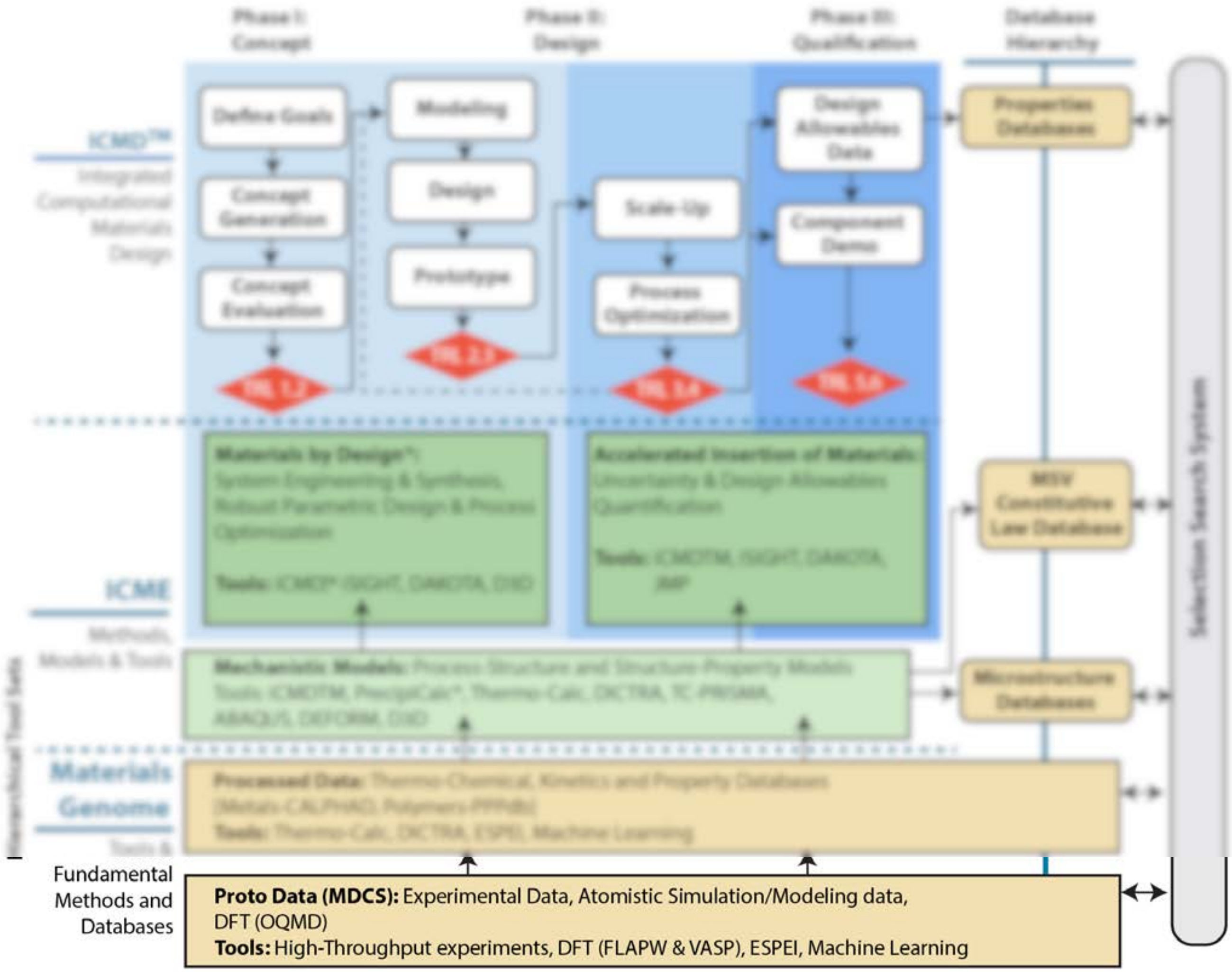
SpaceX metallurgy team developed SX500 superalloy for 12000 psi, hot oxygen-rich gas. It was hard. Almost any metal turns into a flare in those conditions.

7:40 PM - 22 Dec 2018

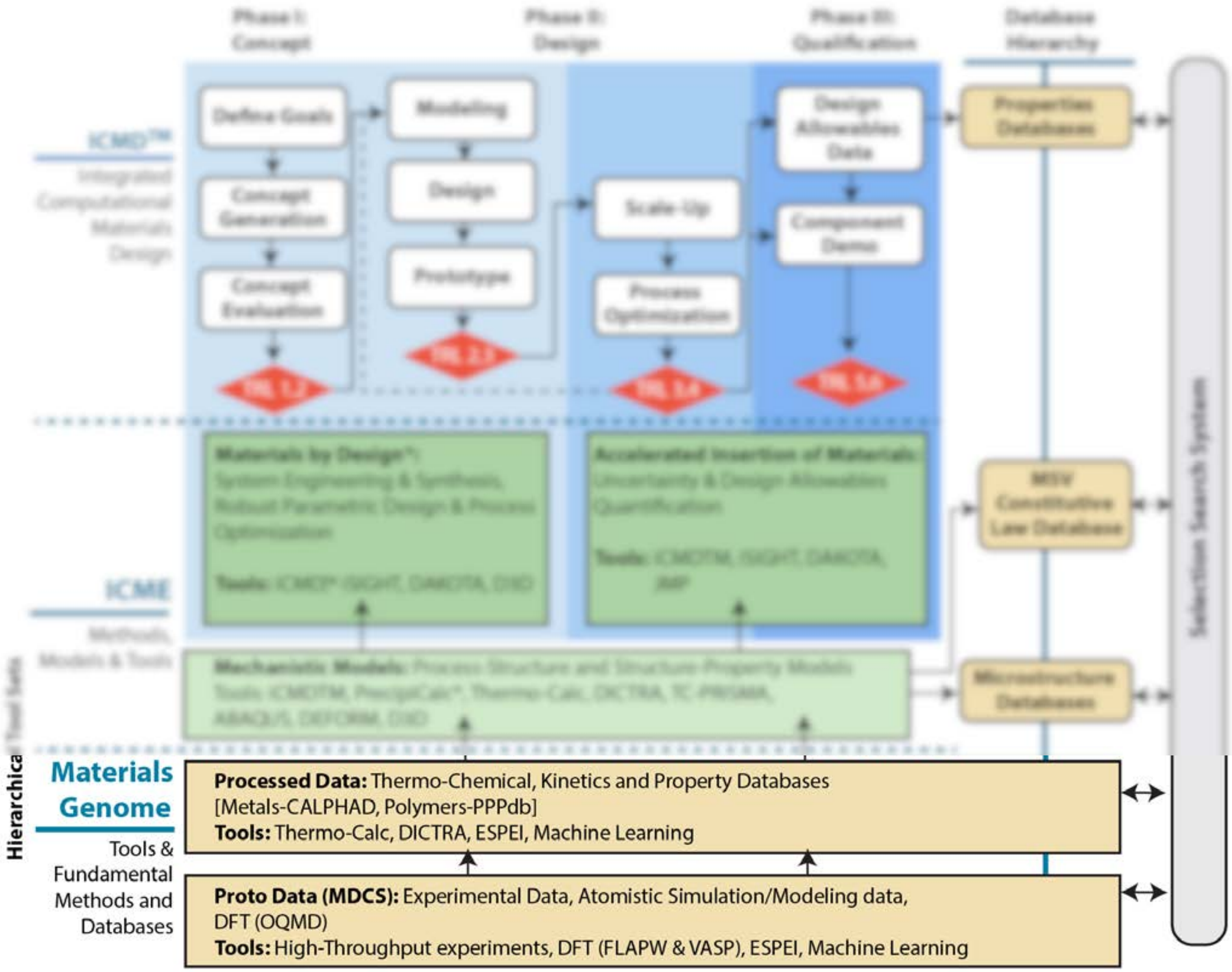
Elon Musk @elonmusk

Three Raptors on a Starship

3:10 PM · Sep 26, 2019 · Twitter for iPhone



Fundamental Methods and Databases
Proto Data (MDCS): Experimental Data, Atomistic Simulation/Modeling data, DFT (OQMD)
Tools: High-Throughput experiments, DFT (FLAPW & VASP), ESPEI, Machine Learning


Materials Genome
Tools & Fundamental Methods and Databases
Hierarchical
Processed Data: Thermo-Chemical, Kinetics and Property Databases
[Metals-CALPHAD, Polymers-PPPdb]
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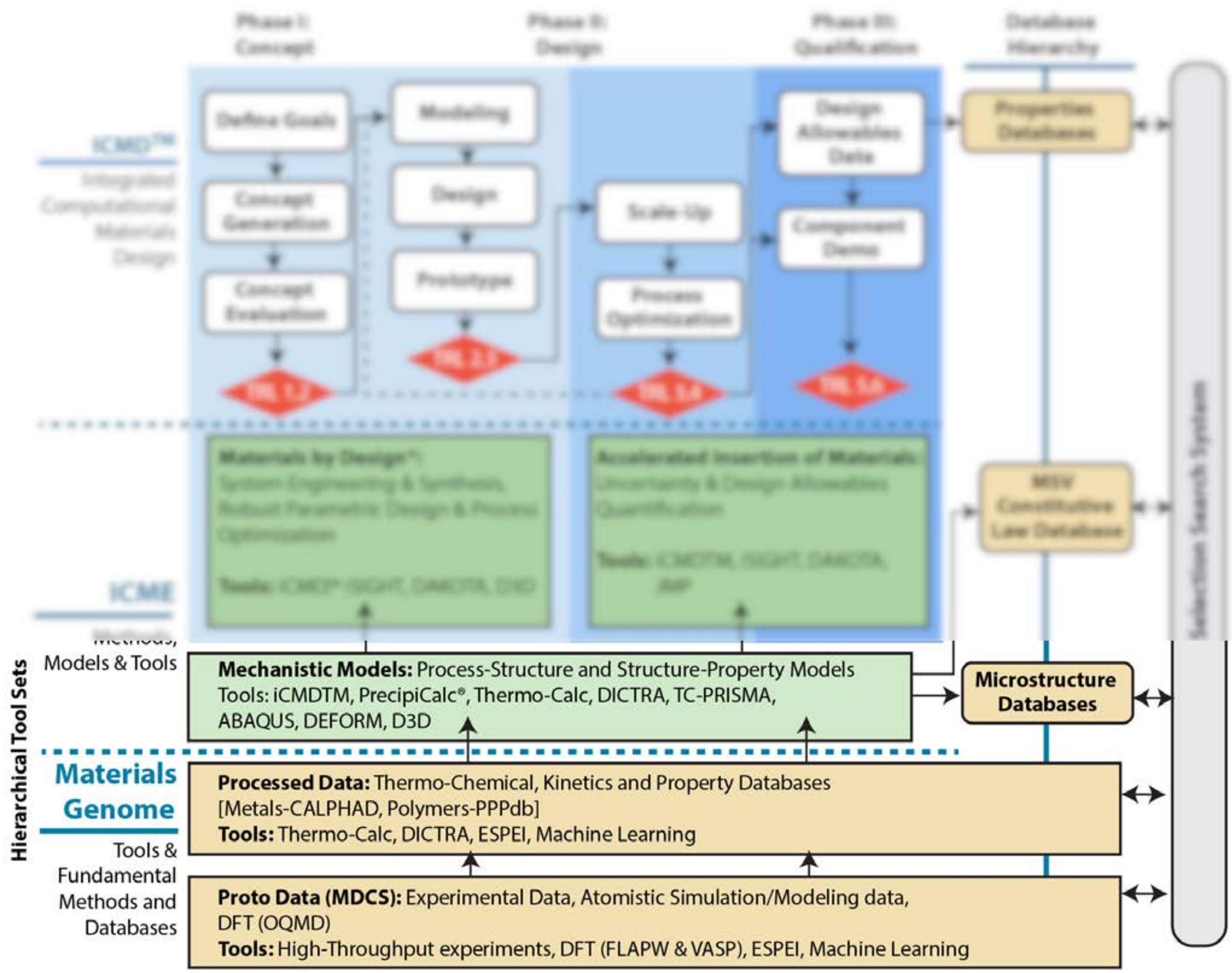
CHiMaD


Hierarchical Tool Sets
Models & Tools
Mechanistic Models: Process-Structure and Structure-Property Models
Tools: iCMDTM, PrecipiCalc®, Thermo-Calc, DICTRA, TC-PRISMA, ABAQUS, DEFORM, D3D
Microstructure Databases
Materials Genome
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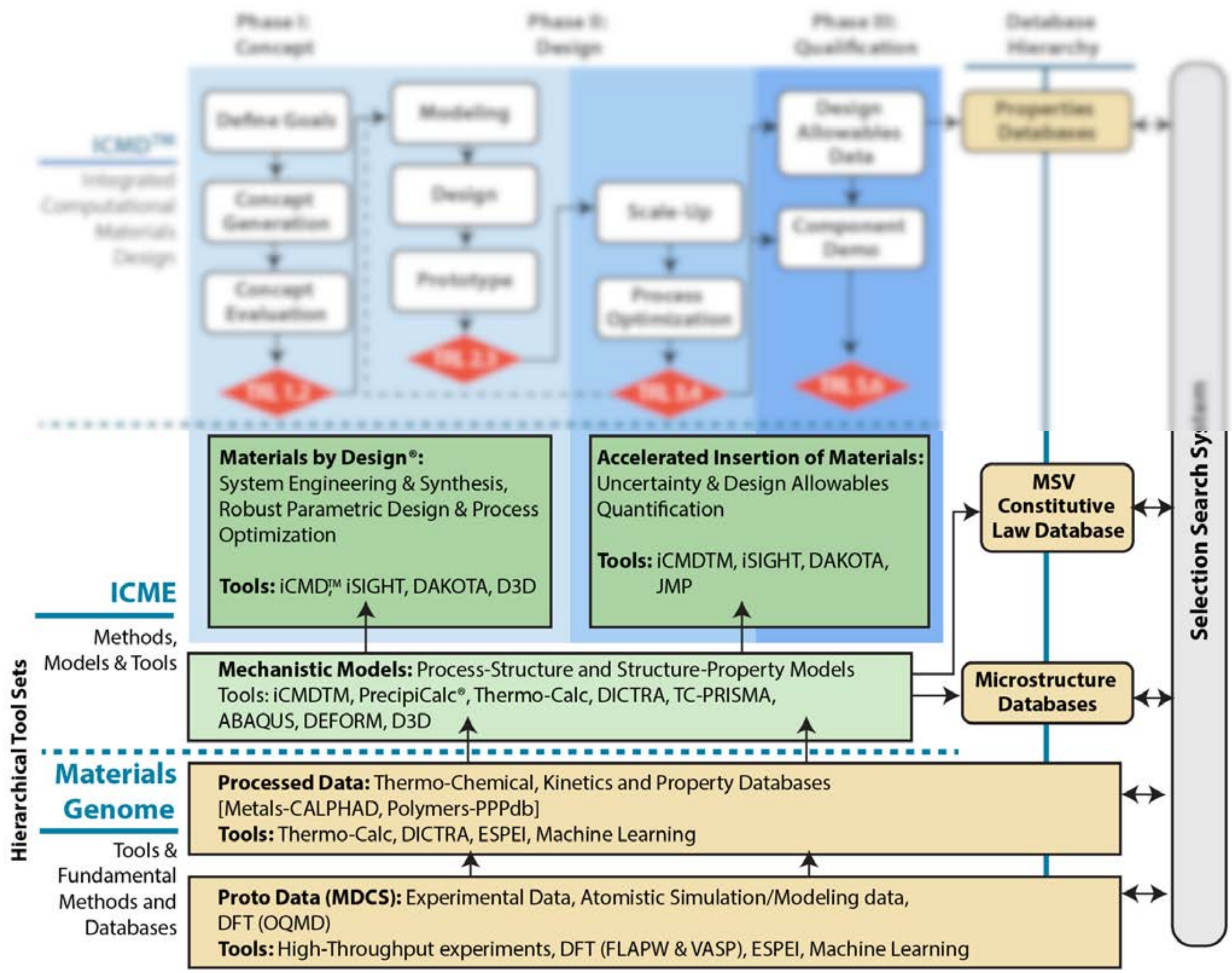
Materials by Design®:
System Engineering & Synthesis, Robust Parametric Design & Process Optimization
Tools: iCMD™ iSIGHT, DAKOTA, D3D
Accelerated Insertion of Materials:
Uncertainty & Design Allowables Quantification
Tools: iCMDTM, iSIGHT, DAKOTA, JMP
ICME
Methods, Models & Tools
Mechanistic Models: Process-Structure and Structure-Property Models
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MSV Constitutive Law Database
Microstructure Databases
Selection Search Sy
Hierarchical Tool Sets
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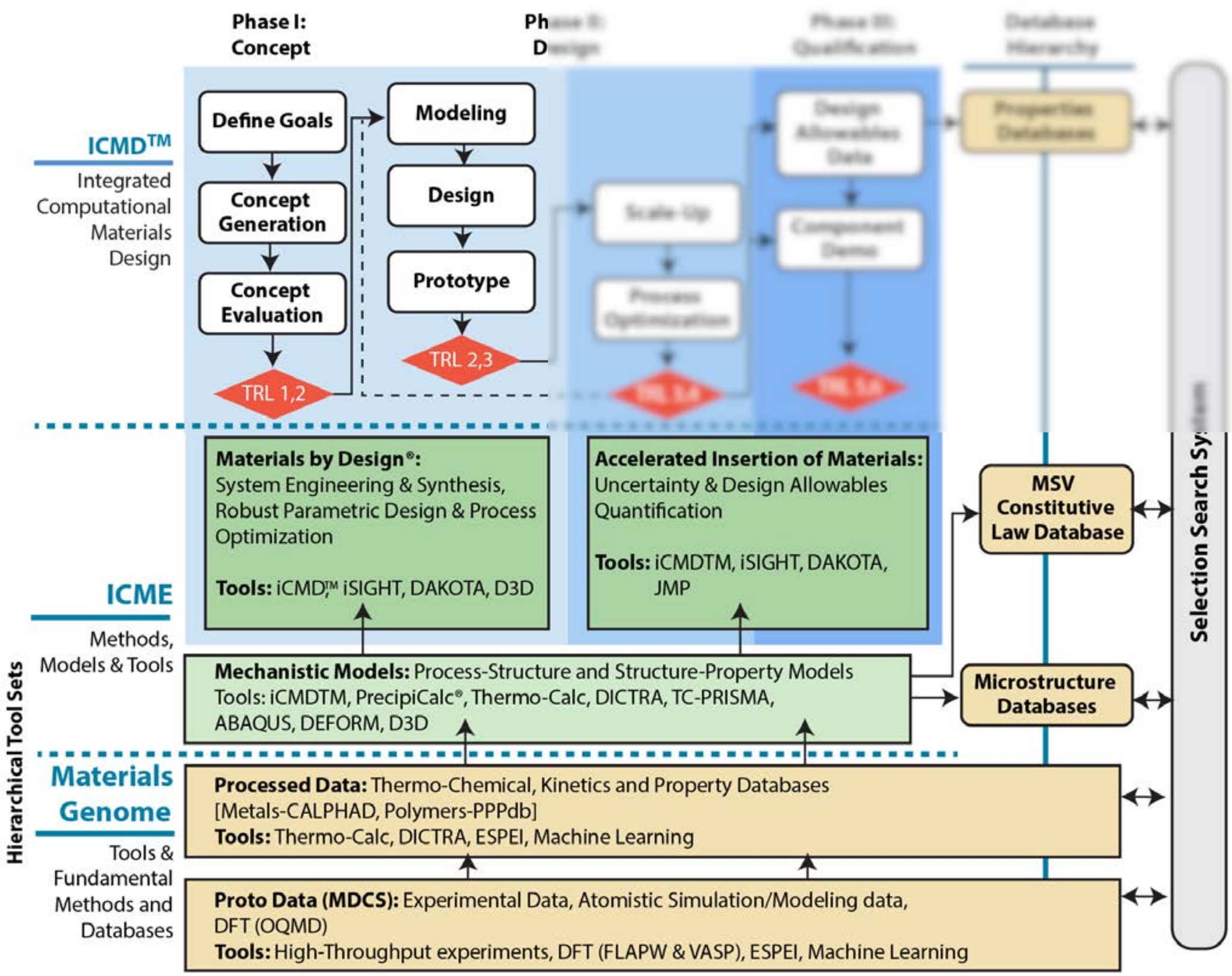

Phase I:
Concept
ICMD™
Integrated Computational Materials Design
Define Goals
Concept Generation
Concept Evaluation
TRL 1,2
Modeling
Design
Prototype
TRL 2,3
ICME
Methods, Models & Tools
Hierarchical Tool Sets
Materials by Design®:
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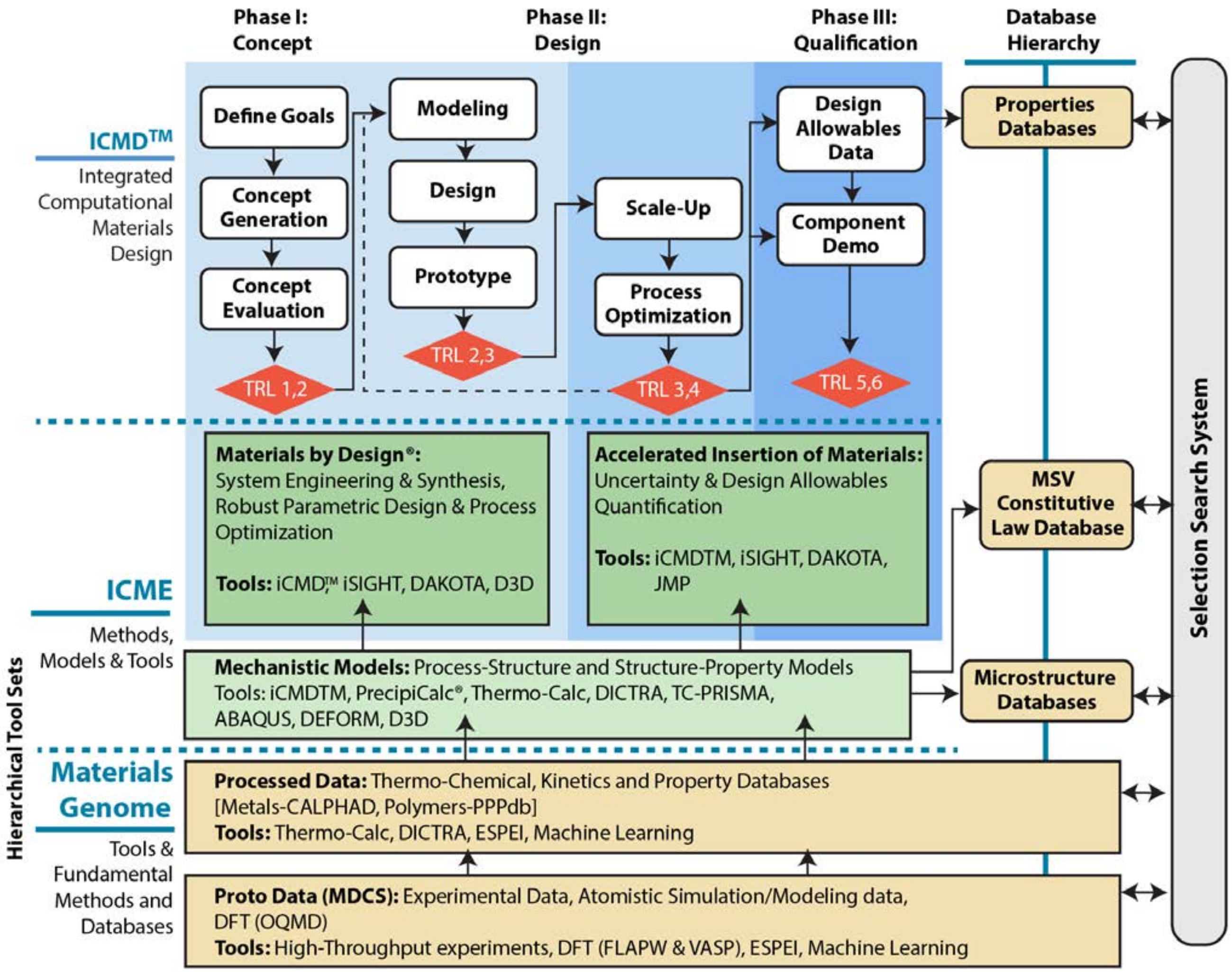
Selection Search

CHiMaD


Phase I: Concept
Phase II: Design
Phase III: Qualification
Database Hierarchy
ICMD™
Integrated Computational Materials Design
Define Goals
Concept Generation
Concept Evaluation
TRL 1,2
Modeling
Design
Prototype
TRL 2,3
Scale-Up
Process Optimization
TRL 3,4
Design Allowables Data
Component Demo
TRL 5,6
Properties Databases
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Selection Search System

CHiMaD

RESEARCH PHASE II

STRUCTURAL MATERIALS

- Alloy Design for Additive Manufacturing
- Co-superalloys for high-temperature use
- Composites for Extreme Environments

FUNCTIONAL MATERIALS

- Grain Boundary and Interface Engineering in Thermoelectrics
- 2D Electronic Material Inks

SOFT MATERIALS

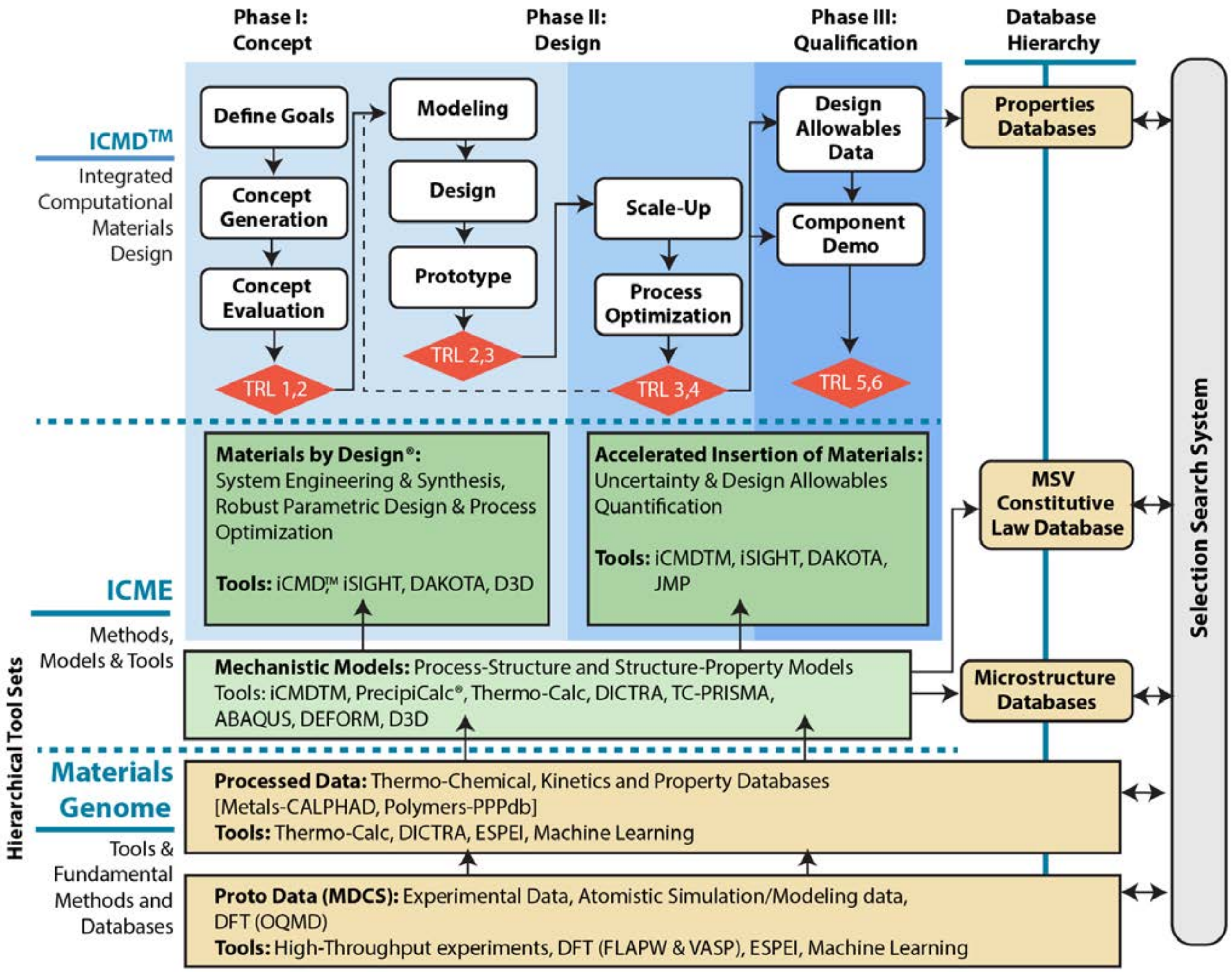
- Directed Self Assembly of Soft Materials
- Design and Properties of Polyelectrolyte Complexes
- High-performance Impact Protection

DESIGN TOOLS

- Phase Field Methods
- Uncertainty Quantification of Phase Equilibria and Thermodynamics

MATERIALS INFORMATICS

- Data Mining and Analytics
- Materials Data Facility


Phase I:
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Materials via Additive Manufacturing

Use localized heating to create novel structures

Aerospace: Fuel Nozzle

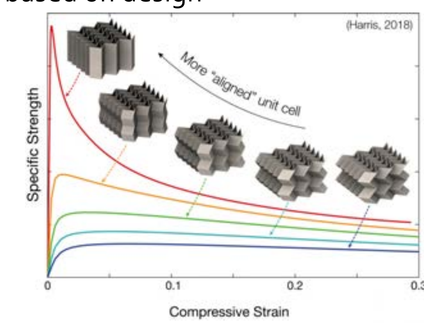
Improved Performance

Medical: Orthopedic Implants

Optimized medical implants based on mechanical response and bone ingrowth

Architected Materials

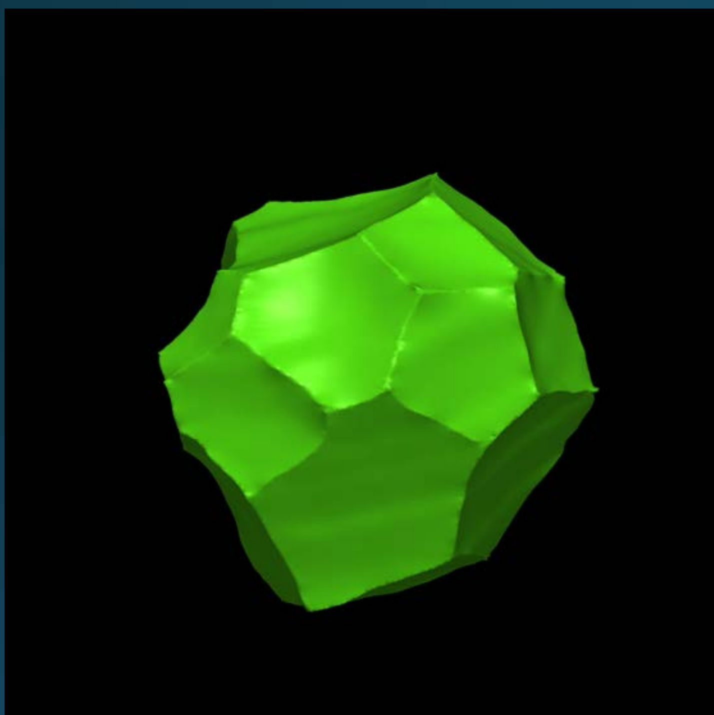
Materials that vary anisotropy based on design



https://youtu.be/qwnzXPb5EKk

Grain Morphologies

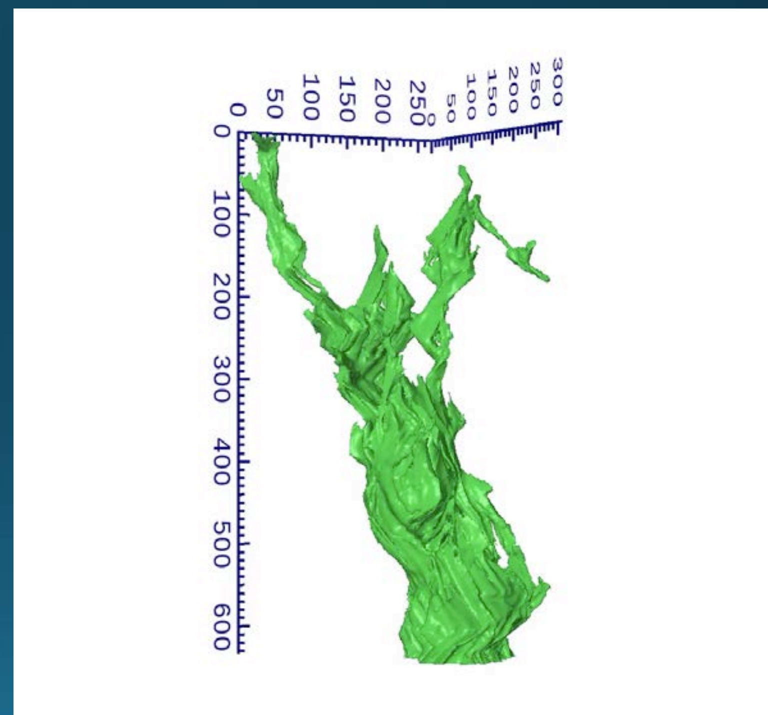
Bulk Processed



Ti-21S

I.M. McKenna et al, Acta Mater. (2014).

Additively Manufactured

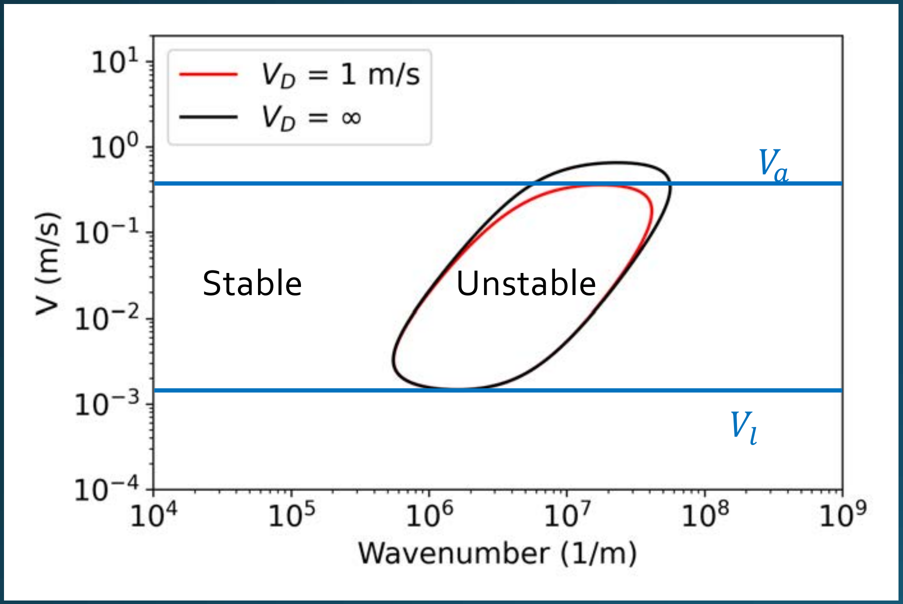


316 L

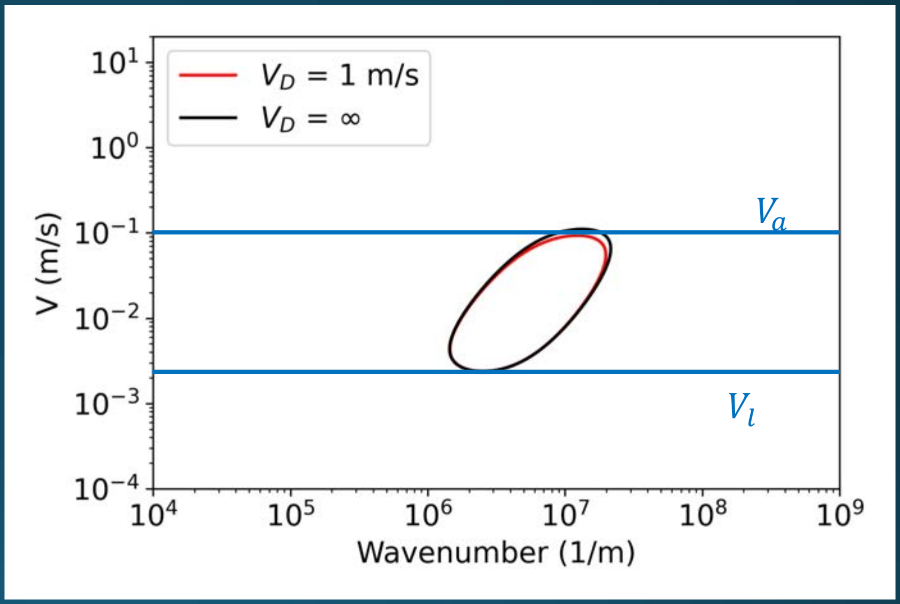
D.W. Rowenhorst et al, Current Op. Solid State, 2020

Rapid Solidification: Absolute Stability for 316L

Ferrite



Austenite



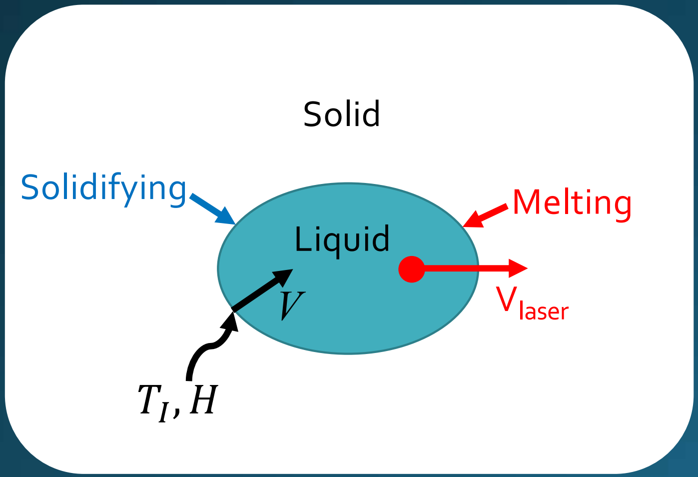
Thermodynamic data courtesy of J. Aroh, C. Pistorius, and A. Rollett (CMU), Mechant and Davis, Acta Mater. 1990

- With increasing interfacial velocity above V_l cells form, then dendrites, then back to cells
- Above V_a the interface is planar

It is likely that the interface is planar or composed of low amplitude cells

Rapid Solidification

- Velocity of laser beam is 10 cm/sec to over 1 m/s
- In the large velocity limit the interfacial velocity is related to the undercooling at the interface



$$V = \mu(T_L - T_I) - \mu\Gamma H$$

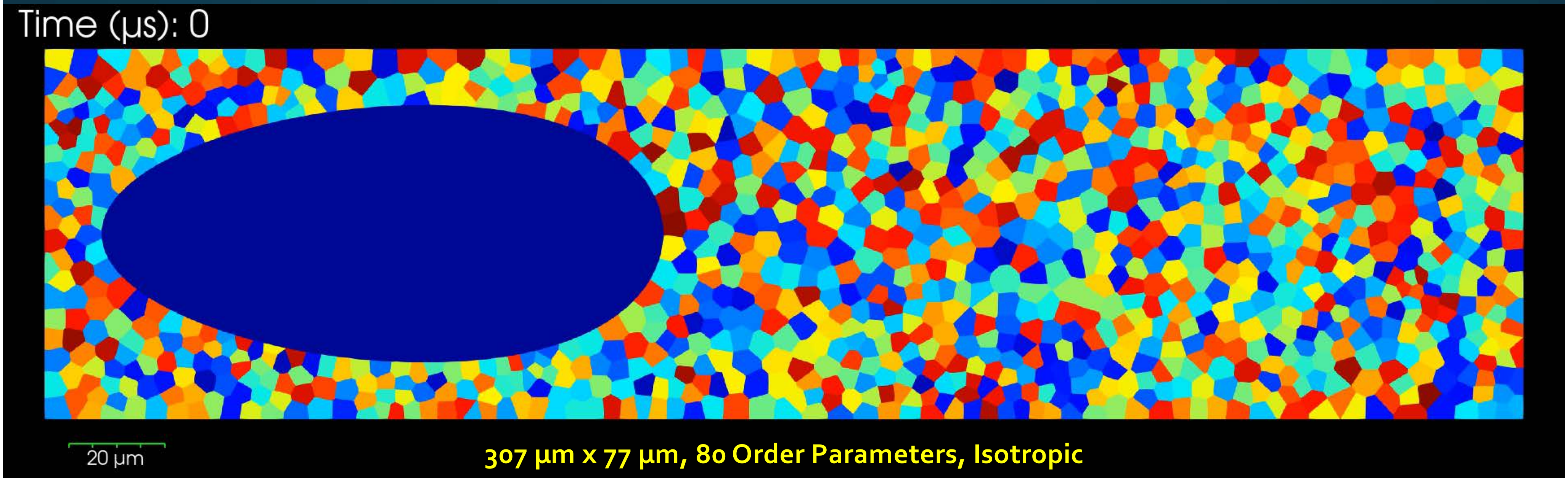
Phase Field Method for AM

- Modify existing multiphase field models to include driving force from local undercooling

$$\frac{\partial \phi_i}{\partial t} = -L_{AC}(\{\phi\}) \left[W \left(\phi_i^3 - \phi_i + 3\phi_i \sum_{j \neq i} \phi_j^2 \right) - \kappa_{AC} \nabla^2 \phi_i + L \, \frac{T_L - T_I}{T_L} \frac{\partial h(\{\phi\})}{\partial \phi_i} \right]$$

- Simple Rosenthal solution for the temperature field

Baseline 2D Results

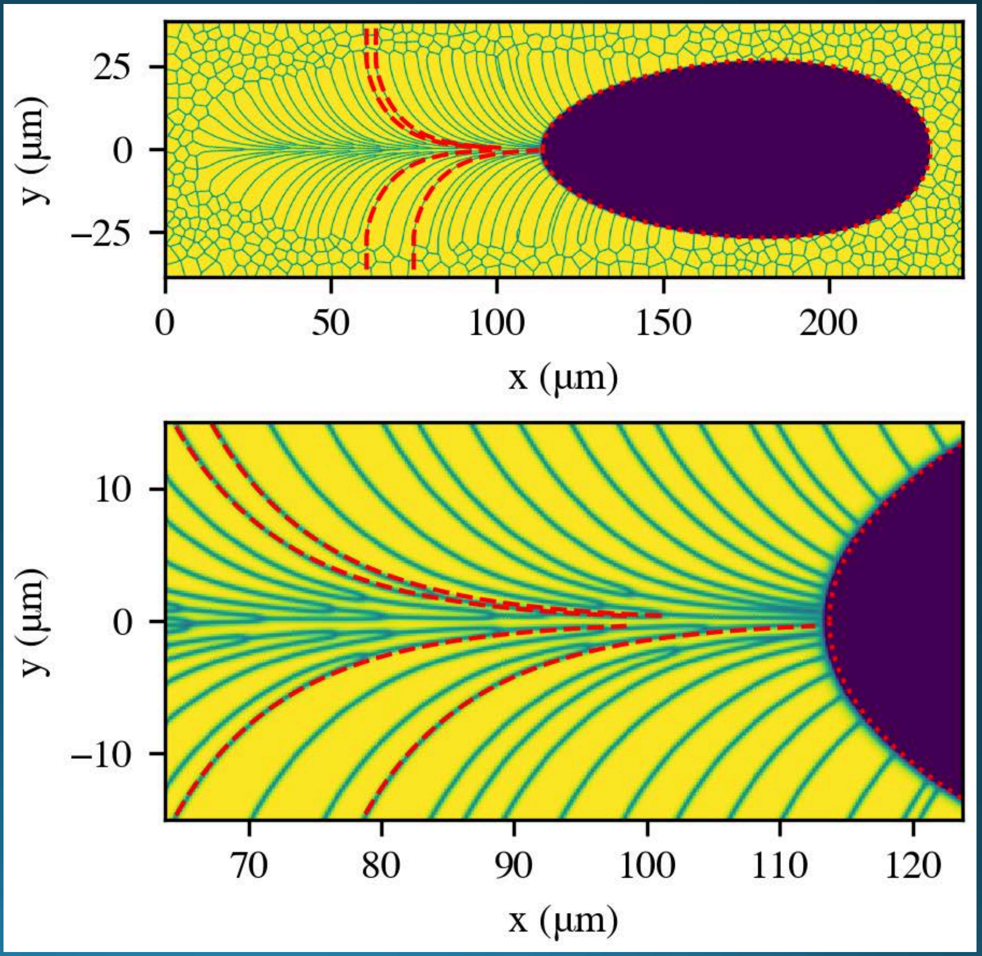


307 μm x 77 μm, 80 Order Parameters, Isotropic

- Grains survive until the centerline: "Infinite" number of grain boundaries
- Trijunctions have nonzero mobilities and grain boundaries remain normal to S/L interface
- Changing normal of the melt pool leads to rotation of the interface

Semianalytical Model

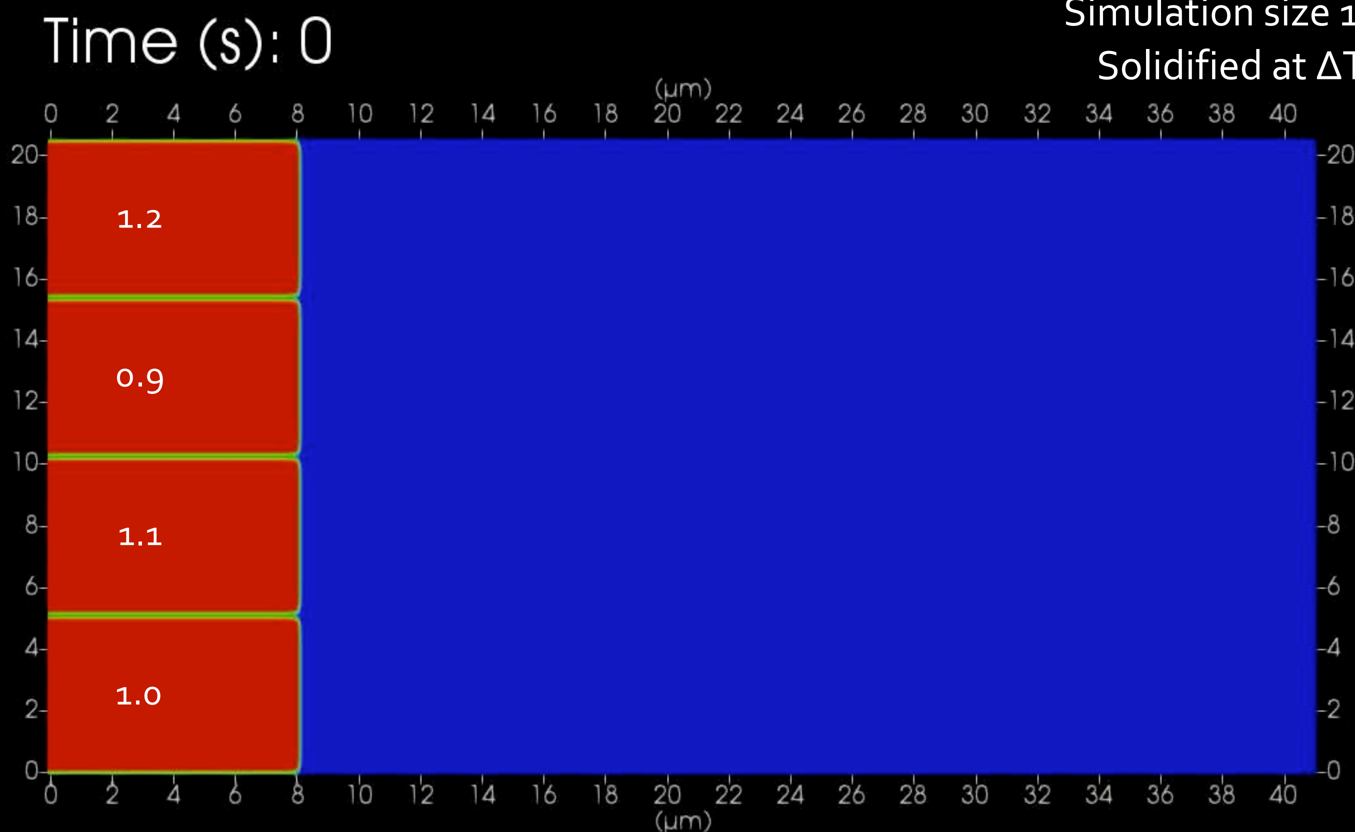
- In the zero interfacial undercooling limit the trijunction remains perpendicular to the liquidus isotherm
- Since we know the temperature field, it is possible write a differential equation for the position of the trijunction as a function of time
- Phase field method is verified
- Curvature induced undercooling stops grain growth at the tips of grains



Competitive growth with varying mobilities

Simulation size 1024 x 2048

Solidified at ΔT = 4.25 K

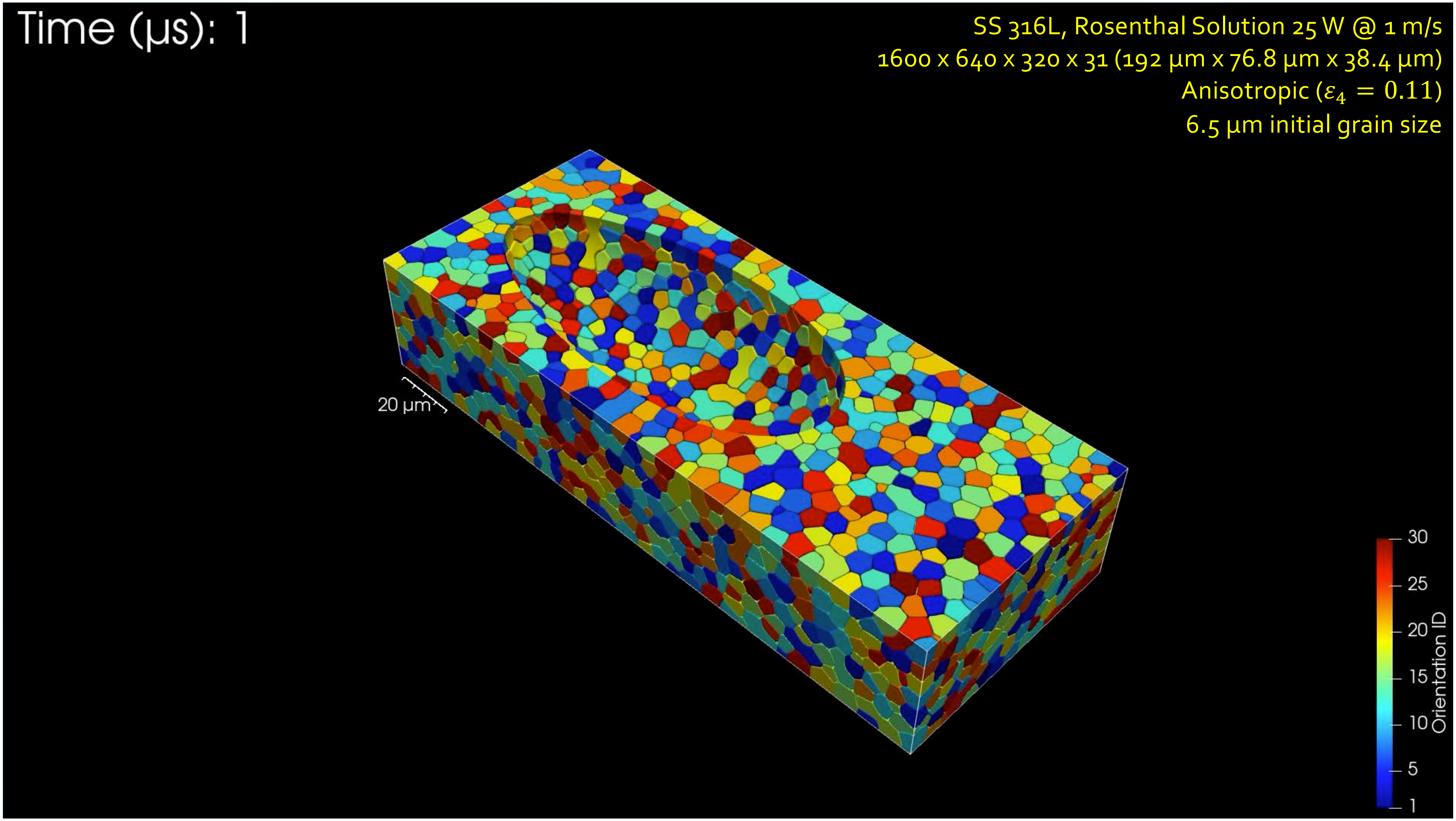


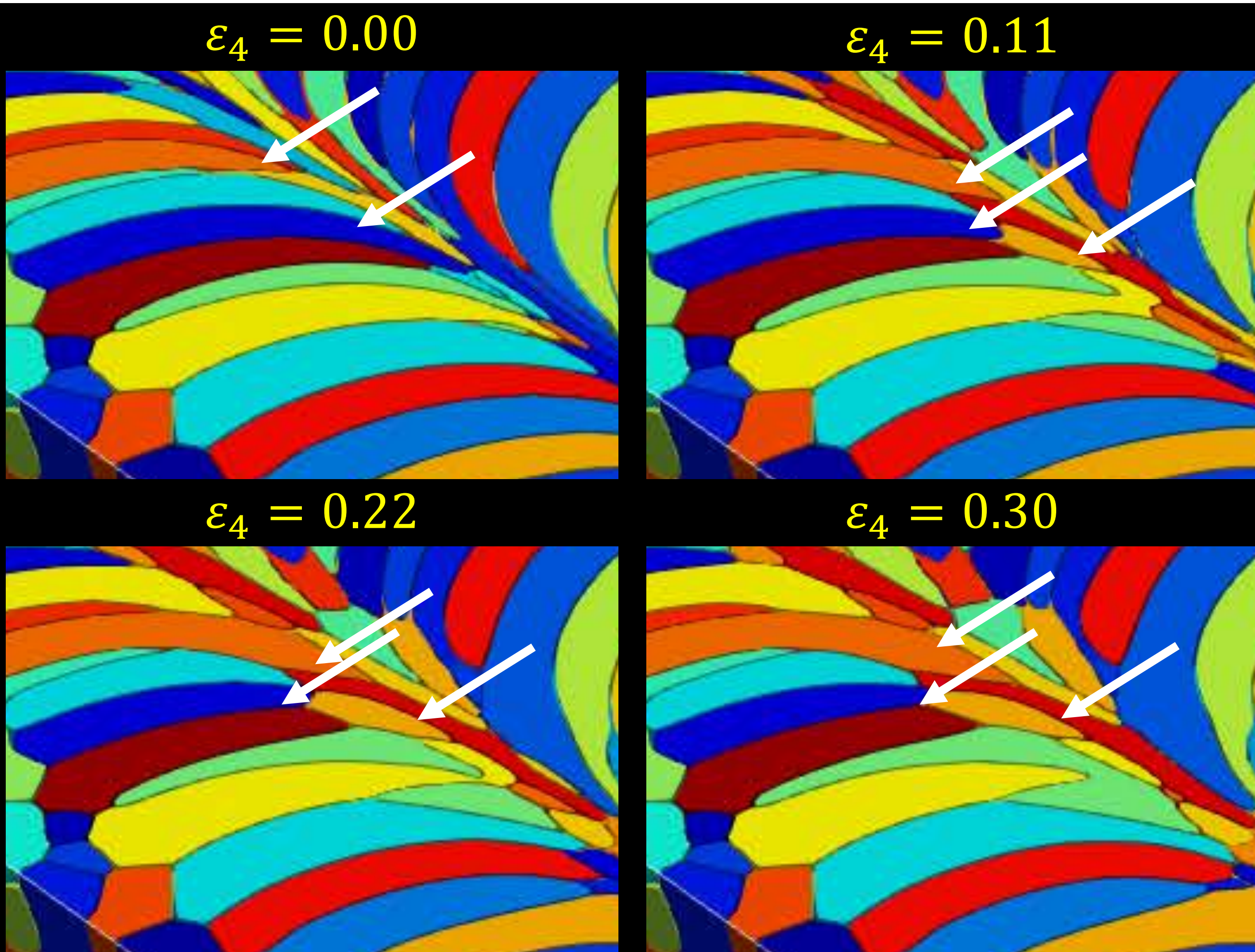
3D Simulations

- Assume an isotropic mobility of the form:

$$L(\boldsymbol{n}) \sim \mu(\boldsymbol{n}) = [1 + \epsilon_4(4(n_1^2 + n_2^2 + n_3^2) - 3)]$$

- Molecular dynamics predicts ε_4 from 0.12 to 0.23
  - The simulations consider ε_4 of 0, 0.11 (reference), 0.22, and 0.3
- Domain is a 192 µm x 77 µm x 38 µm slab, total of 31 order parameters
- Single track typical melt pool width ~160 µm
- Typical runtime: 92 hours on 720 cores
  - Nonlinear transformation of order parameters yields order parameters as quasi distance functions
  - Approximately 2 TB of data per simulation
  - Requires over 2 TB of RAM

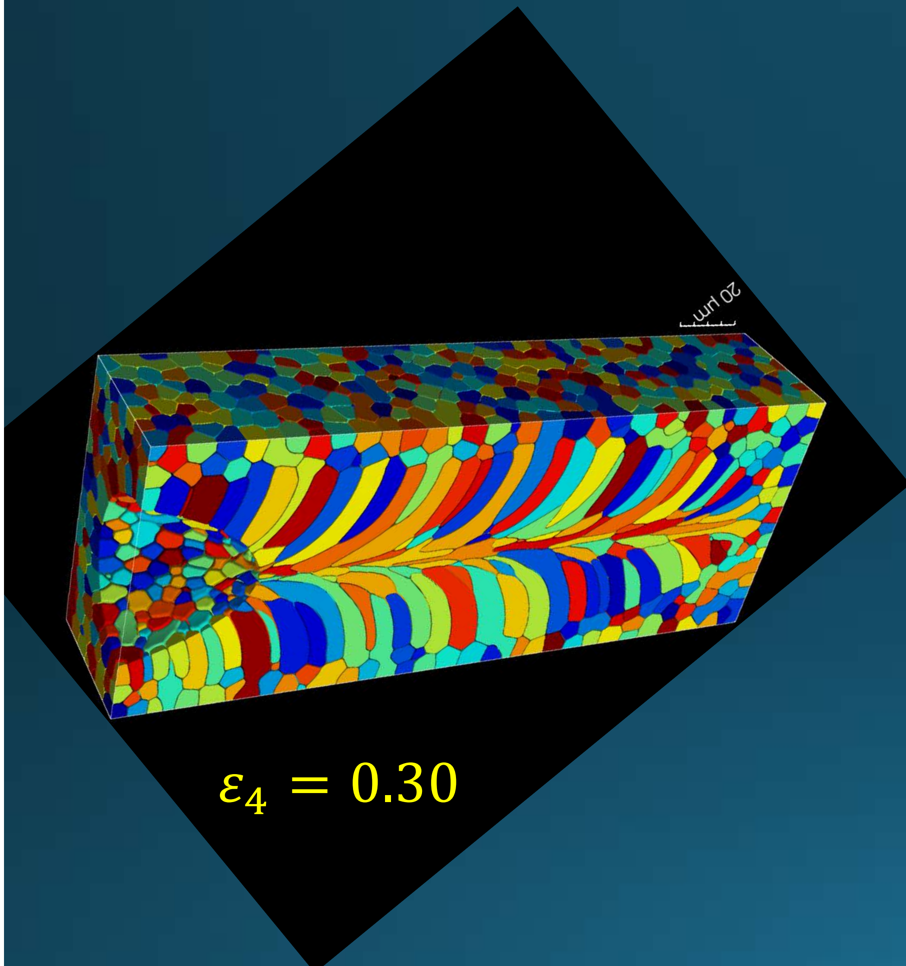

Time (μs): 1
SS 316L, Rosenthal Solution 25 W @ 1 m/s
1600 x 640 x 320 x 31 (192 μm x 76.8 μm x 38.4 μm)
Anisotropic ($\varepsilon_4 = 0.11$)
6.5 μm initial grain size
20 μm
30
25
20
15
10
5
1
Orientation ID

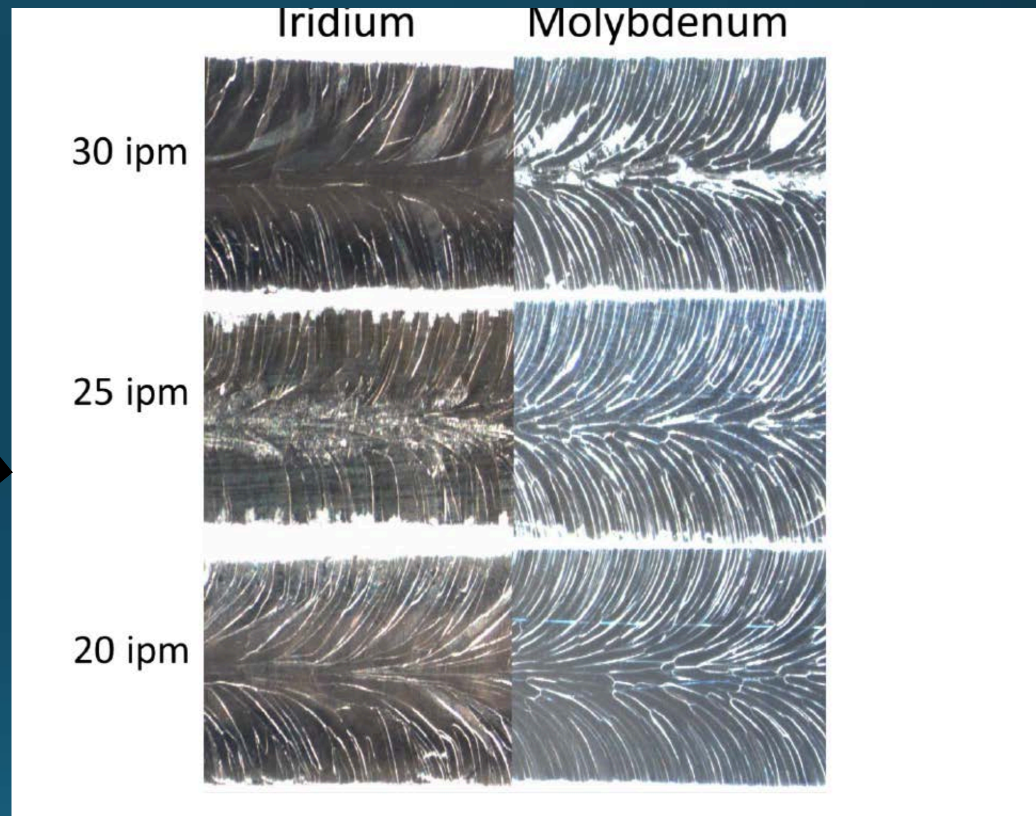


Light blue, dark blue, and brown grains all stop growing well before the center of the melt pool

Orange grain starts to cut off the light blue grain

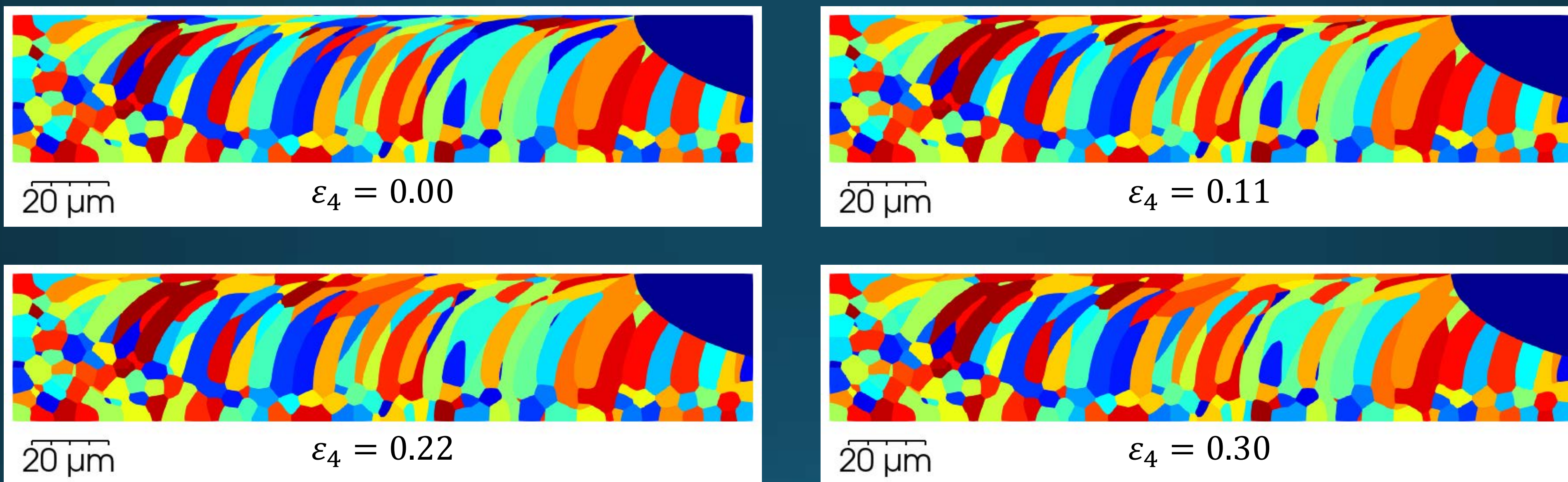
Red and gold grains grew up from below and overtook the blue and brown grains





A. M. Stine, S. W. Pierce, P. F. Moniz, Evaluation of Molybdenum as a Surrogate for Iridium in the 746 GPHS Weld Development, Tech. Rep. LA-UR-15-28088, Los Alamos National Laboratory, Los Alamos,747 NM (Oct. 2015).

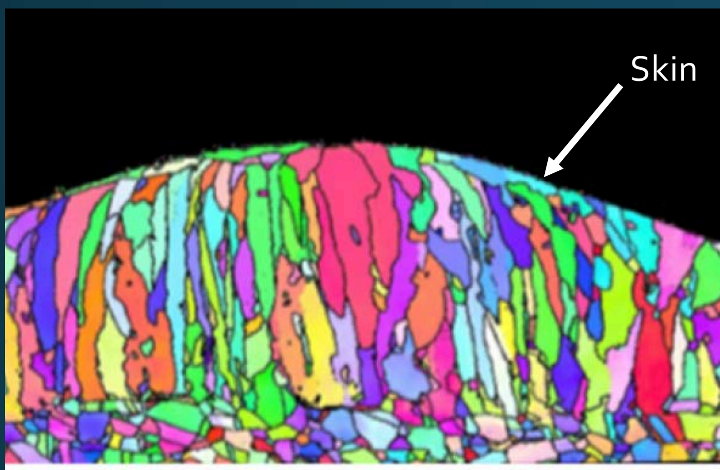
2D Slices Along Laser Path



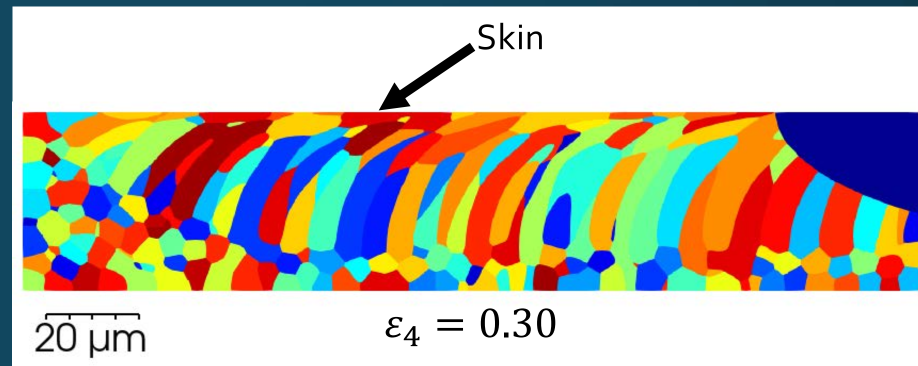
- In 2D slice, "epitaxial" grains appear to grow upright from substrate
- Top skin of small grains grew in from other directions

2D Slices Along Laser Path

316L



Andrew Birnbaum et *Additive Manufacturing* (2019)



- Upright, epitaxial growth and skin layer of small grains qualitatively similar to NRL single track builds