TEXAS A&M UNIVERSITY
High Performance Research Computing

Spotlights: Research Expedited by HPC

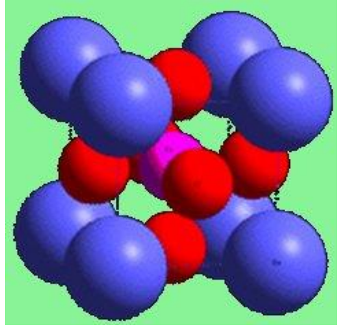
Accelerated Development of Materials, The Future Is Here (!)

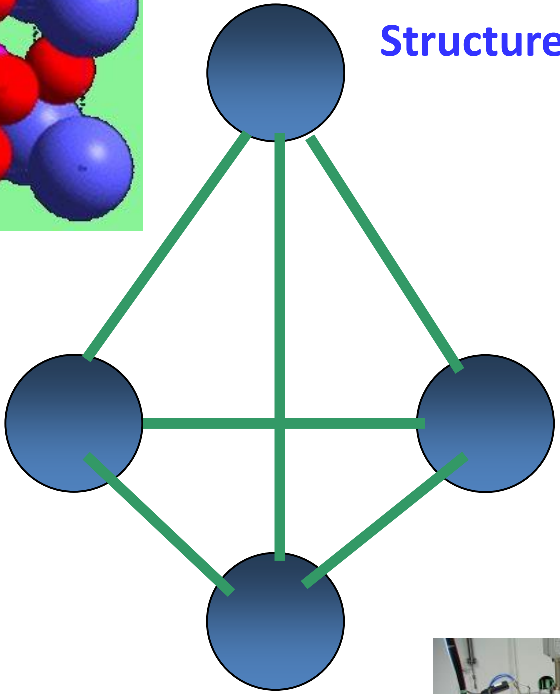
– Raymundo Arróyave

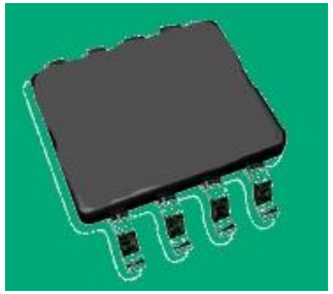
Materials Science and Engineering

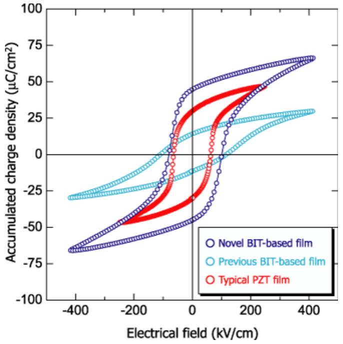
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

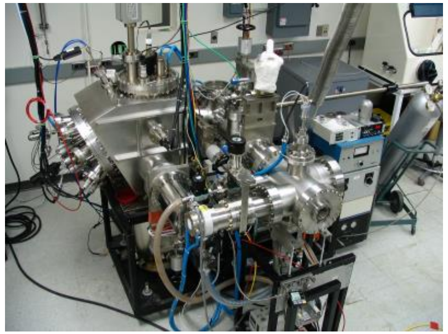
Some Definitions: Materials Science & Engineering





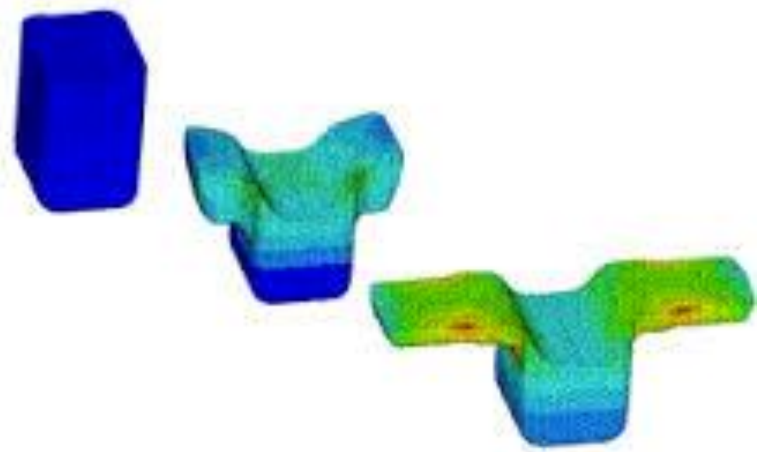






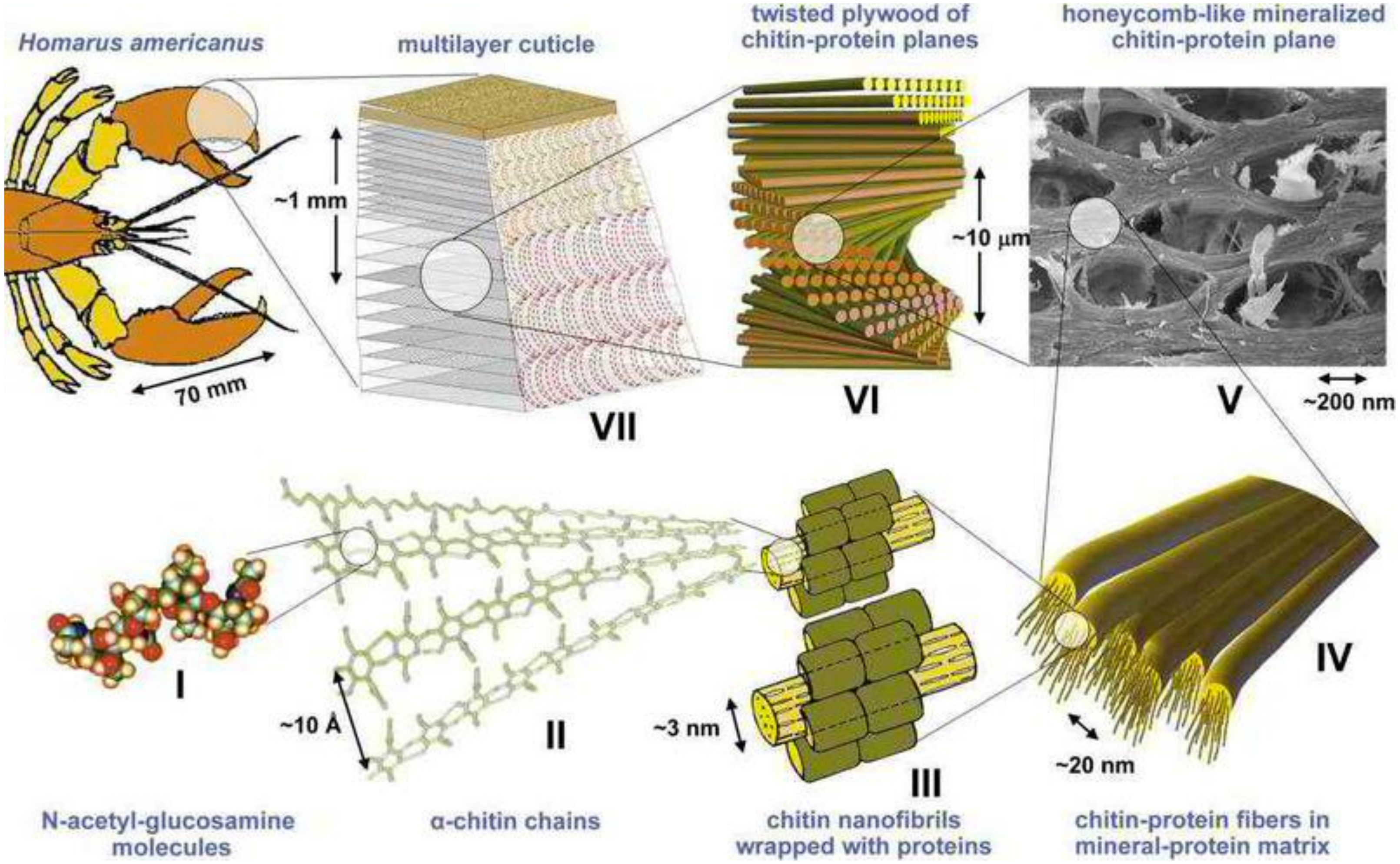
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Some Definitions: Processing



Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

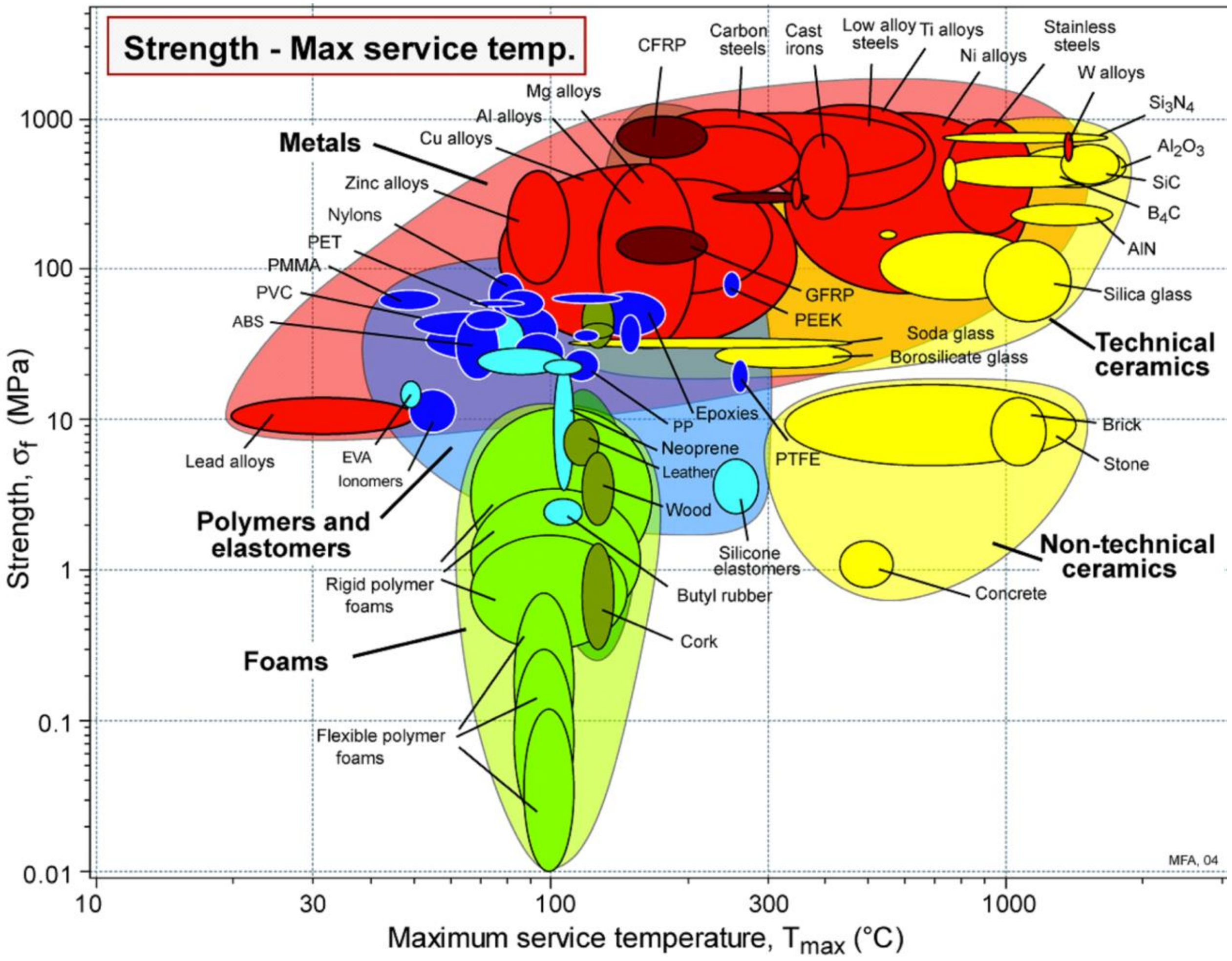
Some Definitions: Structure



http://www..dierk-raabe.com/biological-natural-materials/chitin/

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Some Definitions: Properties/Performance

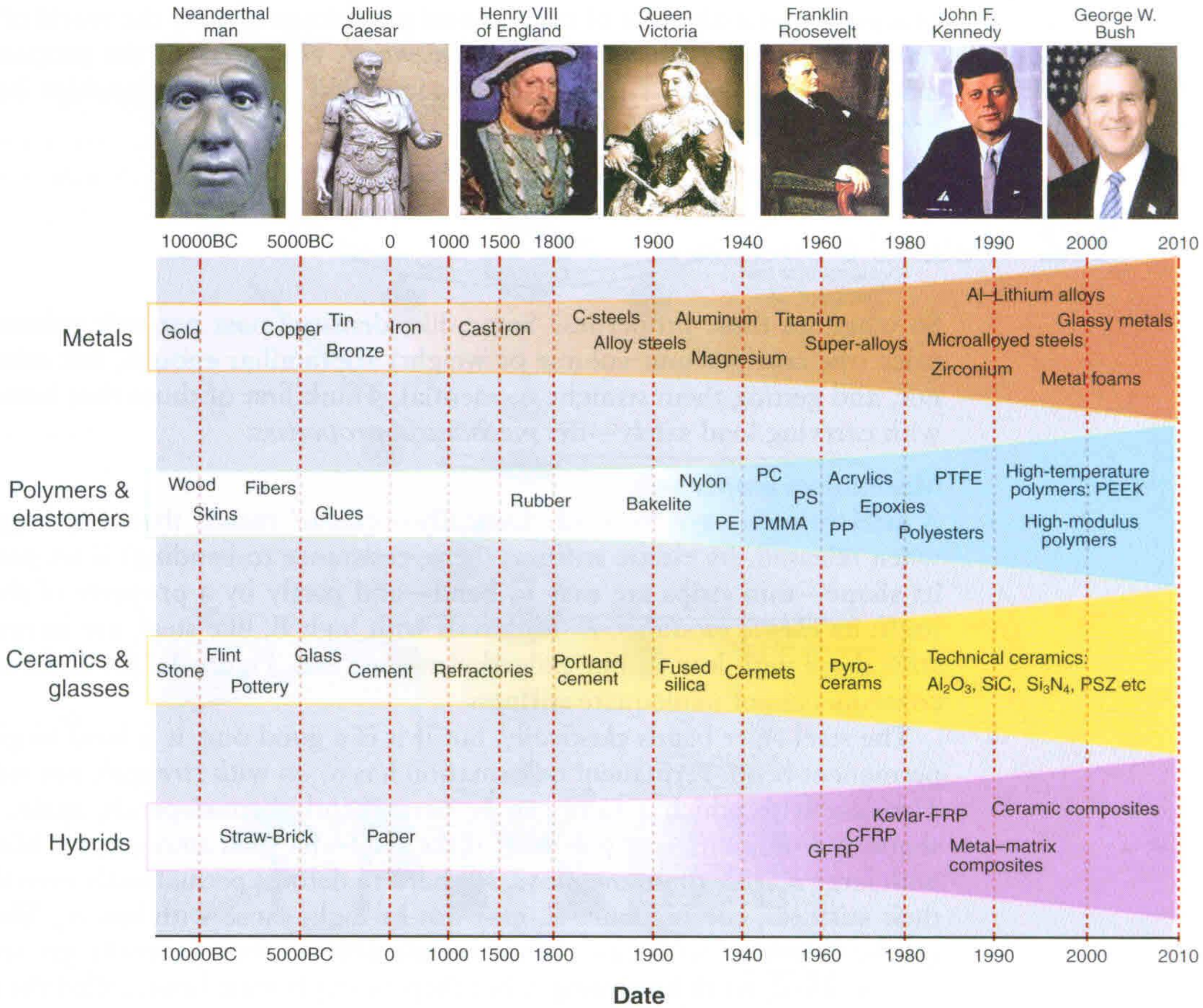


http://www..tangram.co.uk/TI-Polymer-High_temperature_plastics.html

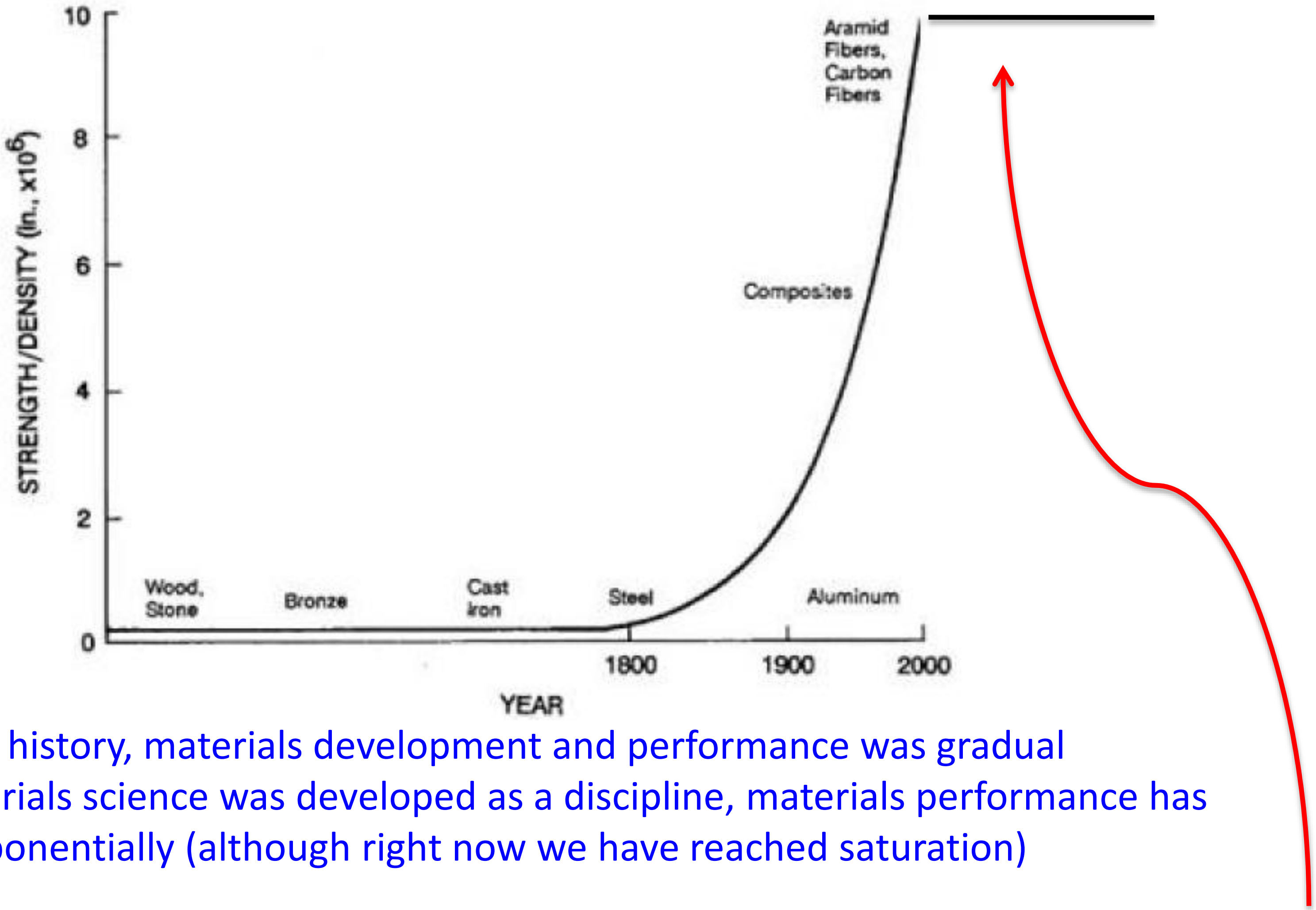
Materials Development

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

A Bit of History: Materials Development through Time



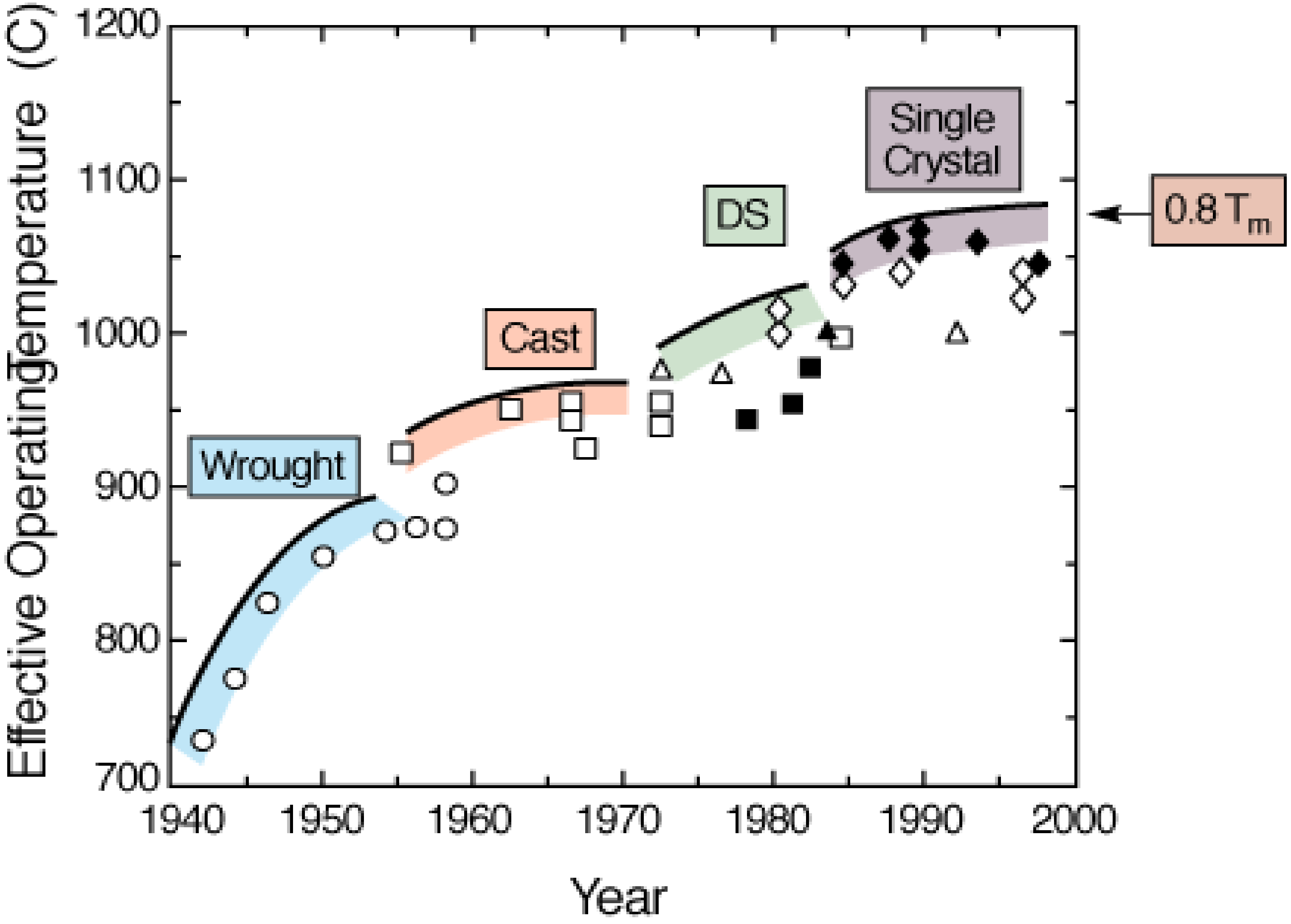
Materials Performance over Time:



- For 99% of history, materials development and performance was gradual
- Once materials science was developed as a discipline, materials performance has evolved exponentially (although right now we have reached saturation)

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Materials Development has reached Saturation in Many Applications:

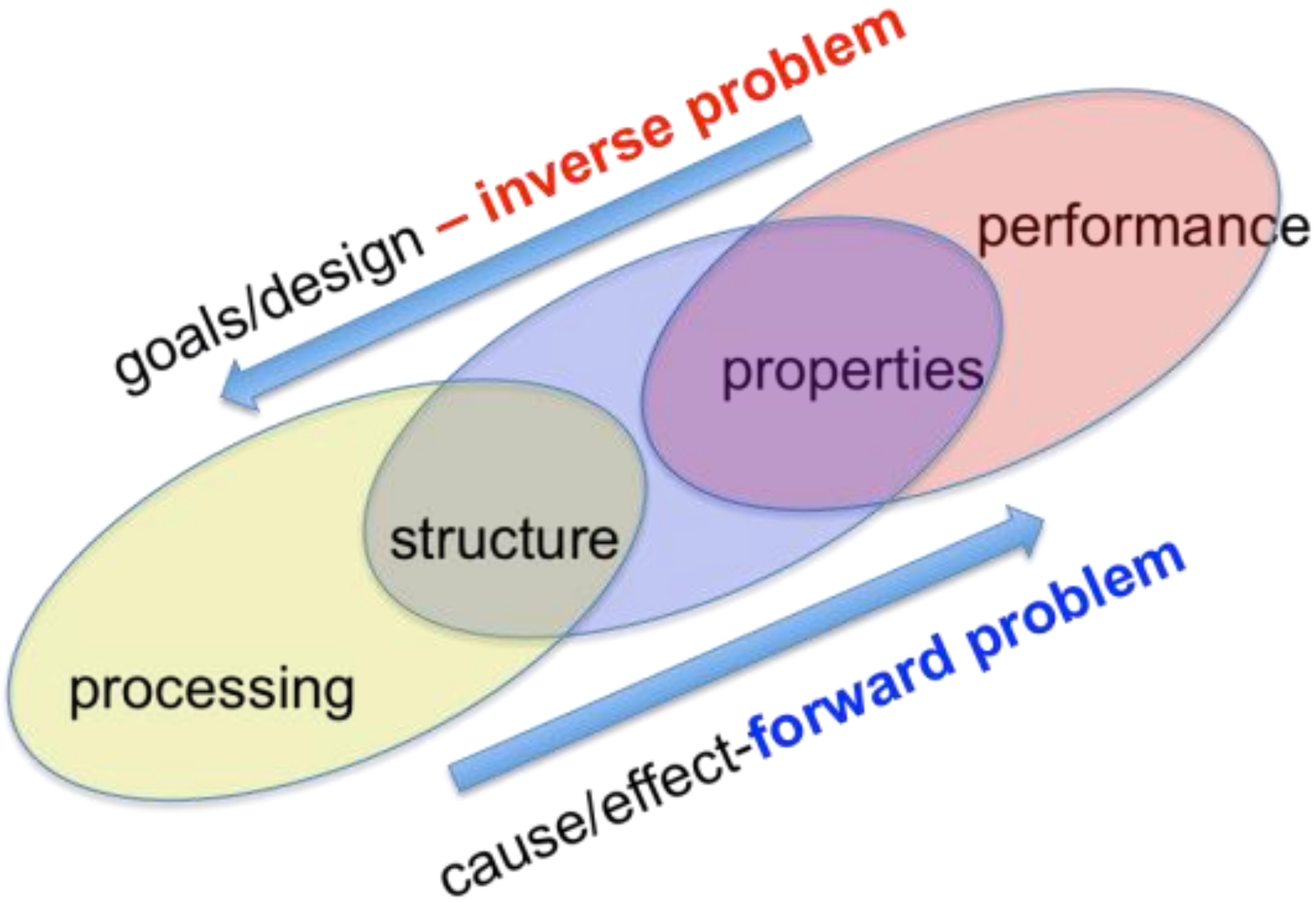


Materials Development

- In prehistory:
  - Materials development is completely accidental
  - ‘Wheel’ is perhaps discovered millions of times
- Antiquity (begining of our civilization):
  - Development of rules and ‘recipes’ based on empirical observation
  - Nice example: ritual followed by master Japanese swordsmiths
- Modern Age:
  - Knowledge is organized/systematized
  - Development of Scientific Method (experiment, observation, development of hypotheses)
  - Recognition of Materials Classes
- Today:
  - Integration of three ‘kinds’ of knowing: experiment, theory, computation (within an informatics framework)

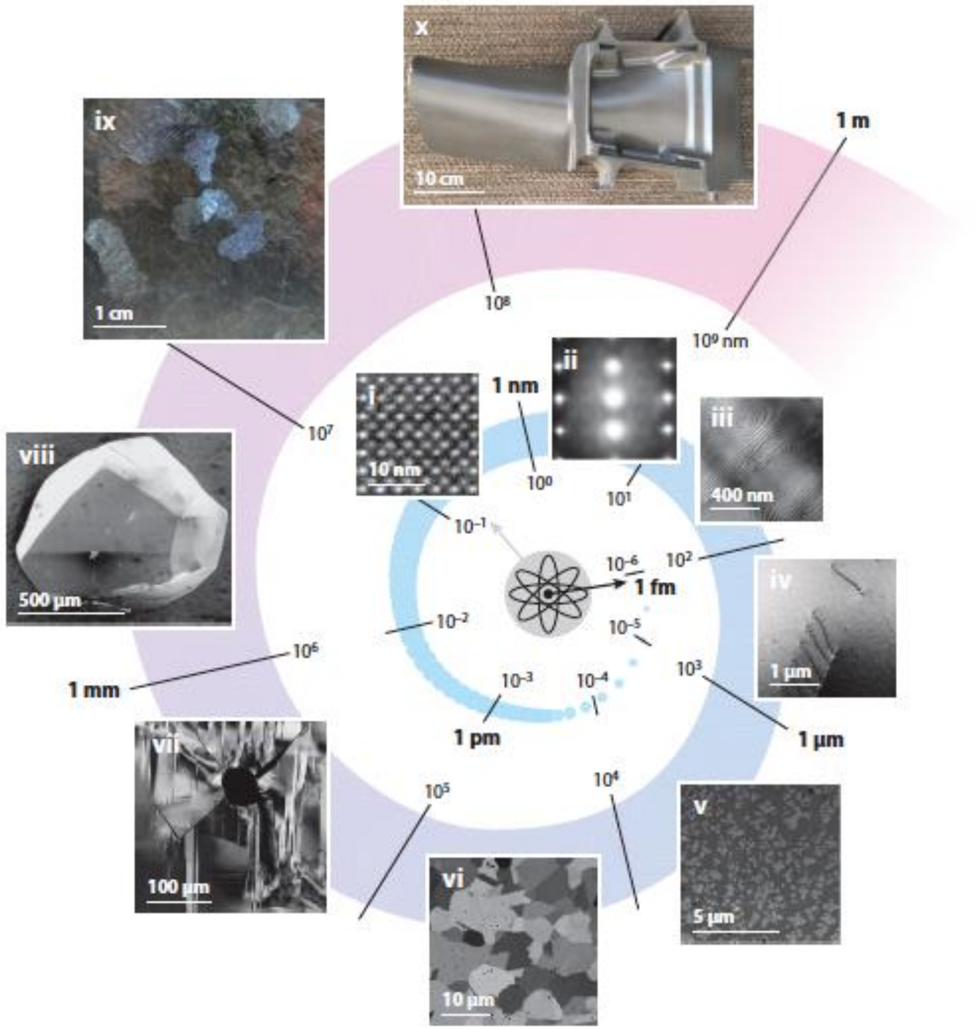
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

What Materials Science is About

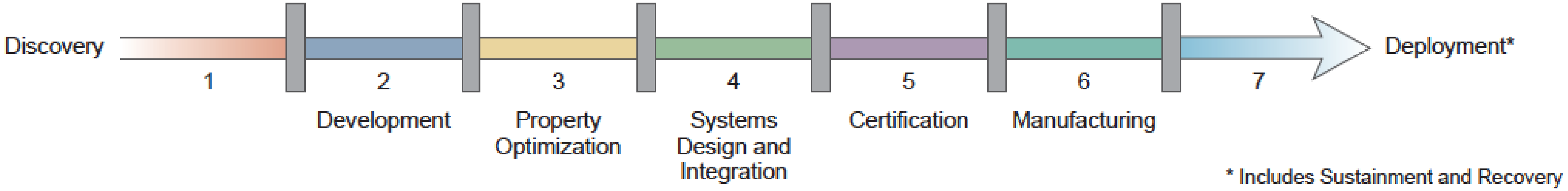


Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

The Challenge: Materials are Multi-Scale Systems!



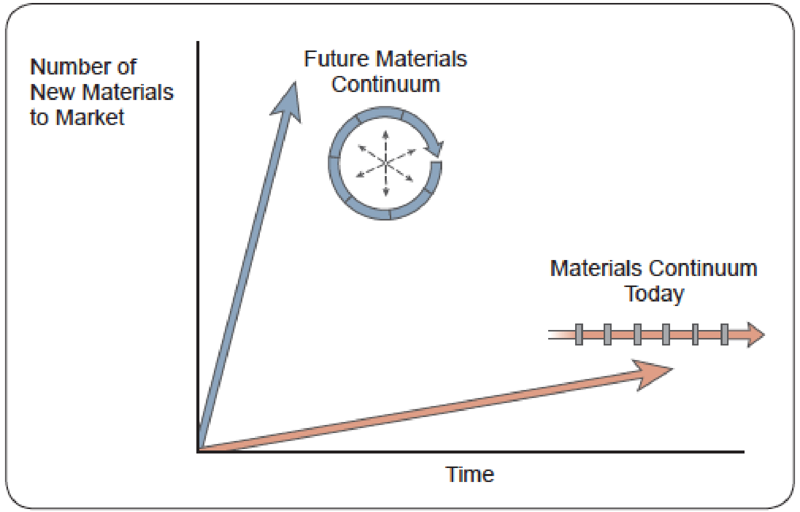
Materials Genome Initiative



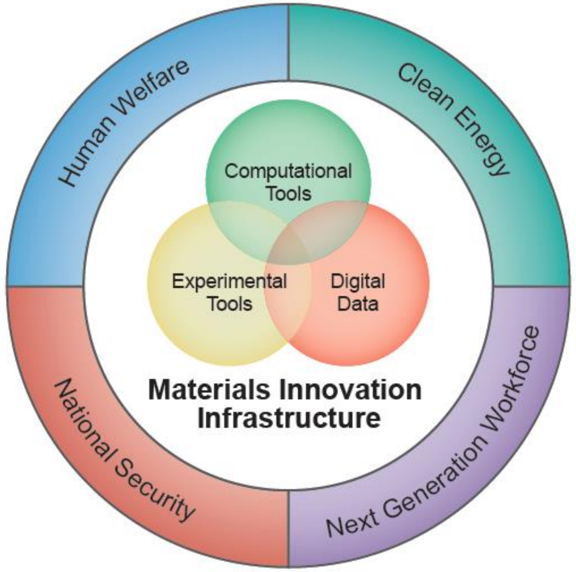
Typical Time Frame ~ 15- 20 years!!!

Current activities:

Goal: Reduce Cost and Time by Half



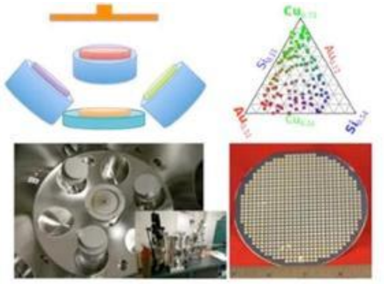
The Materials Genome Initiative:



Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

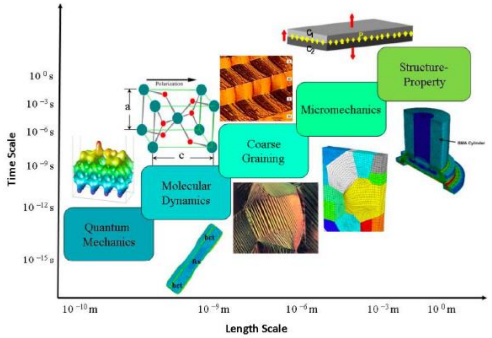
Materials Genome Initiative

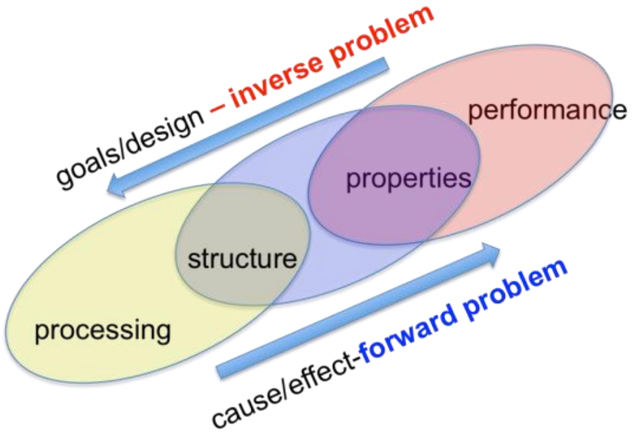
High-throughput Computation/Experiments



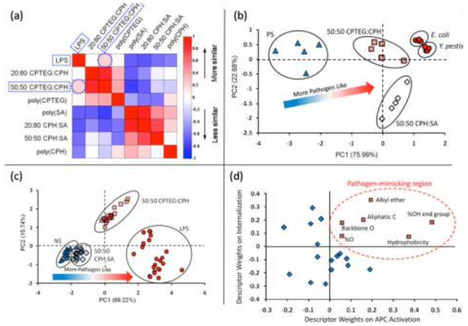
SPS, PVD
High-Performance Computing

Multi-Scale Modeling

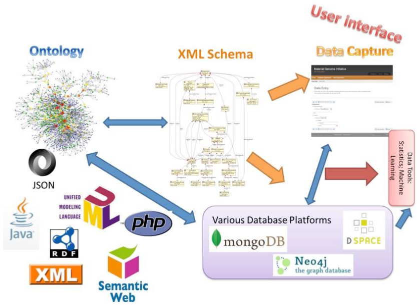




Materials Informatics



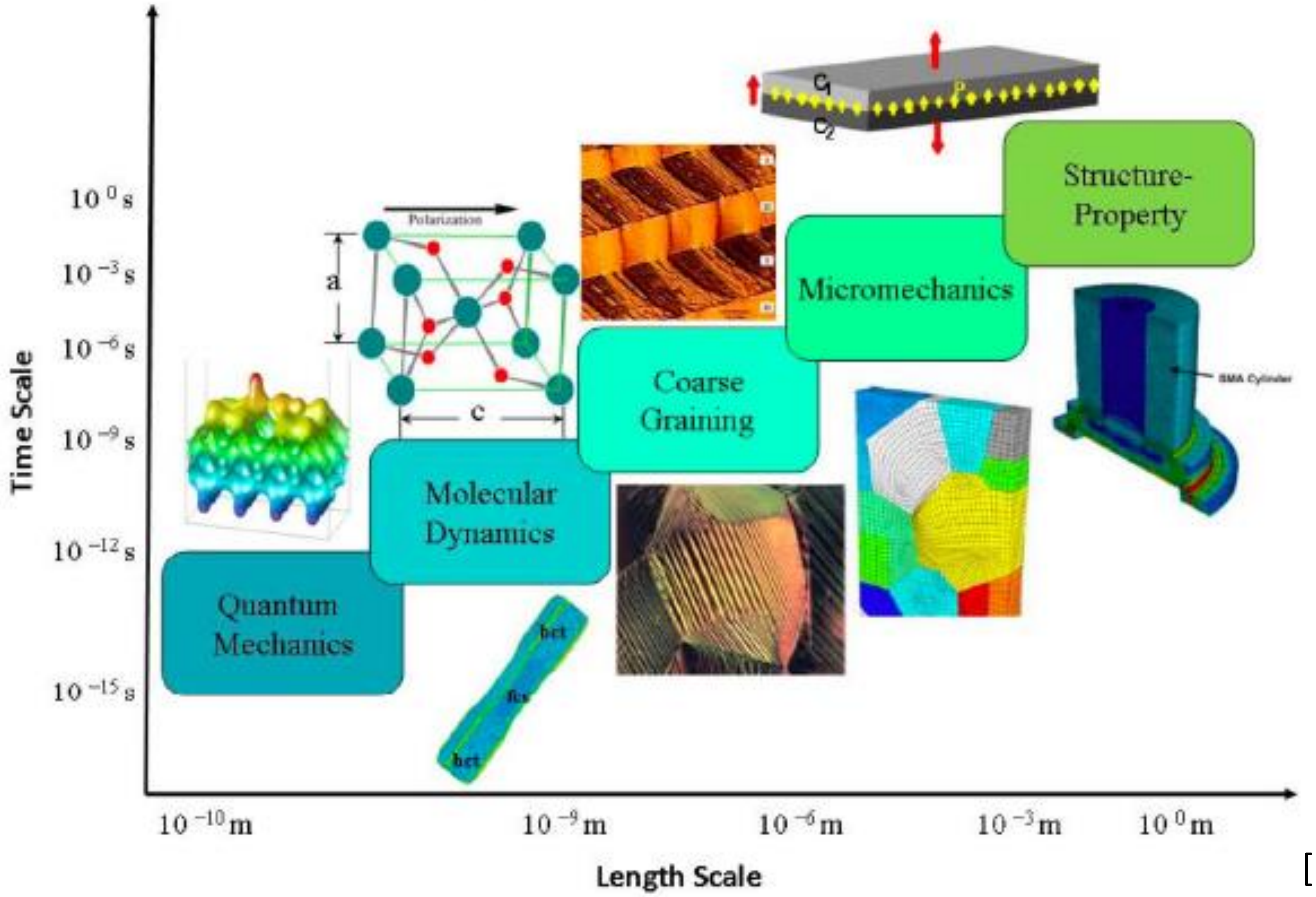
Database Development



Multi-Scale Modeling

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Multi-Scale Computational Materials Science

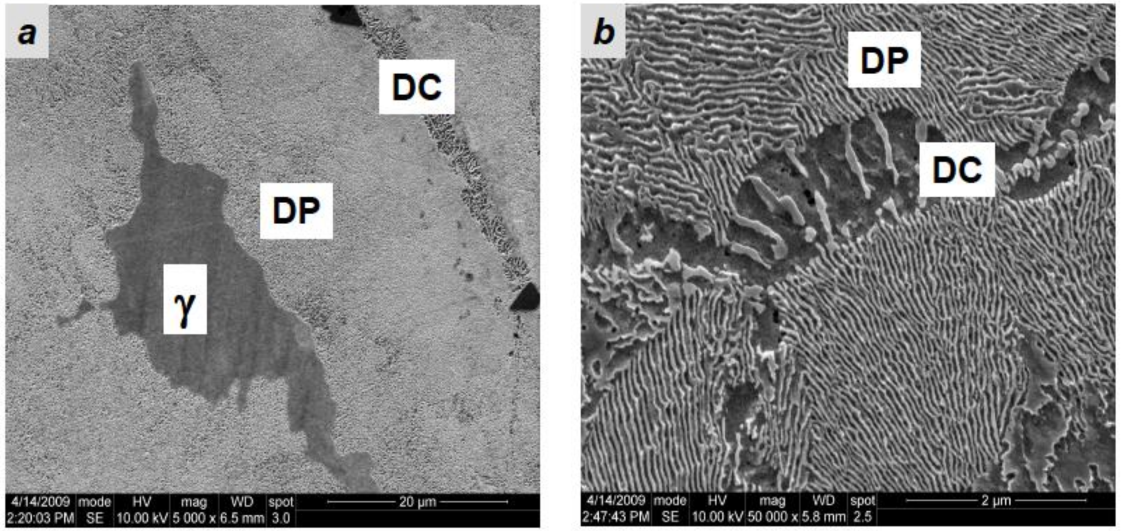


[Lagoudas]

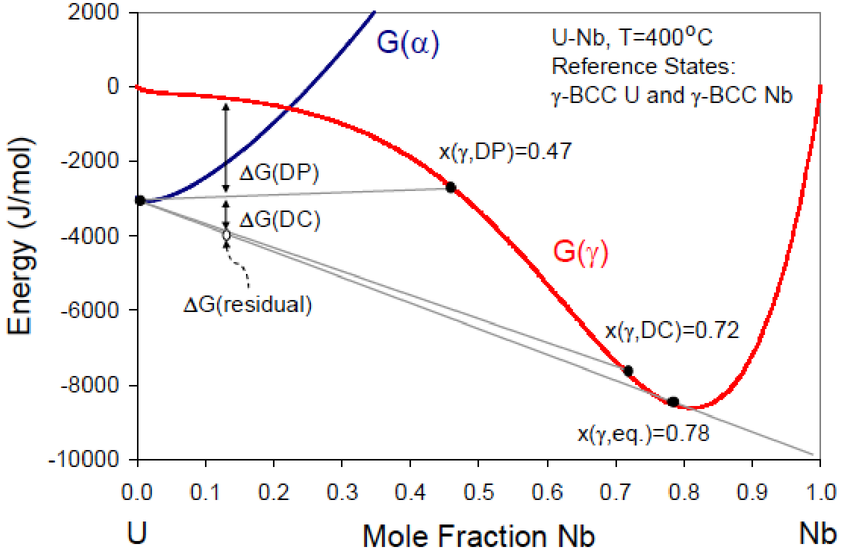
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Multi-scale Modeling Example: Discontinuous Precipitation

From DFT to Microstructure Evolution:
Discontinuous Precipitation in Metallic Alloys



Alloy trapped in metastable states:

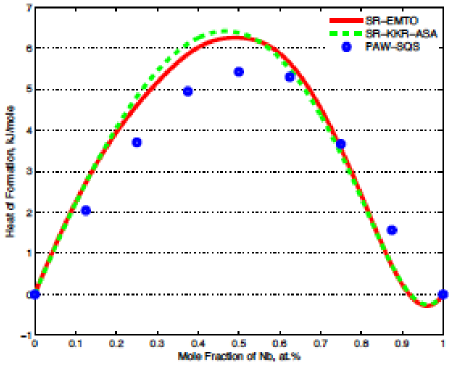


Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

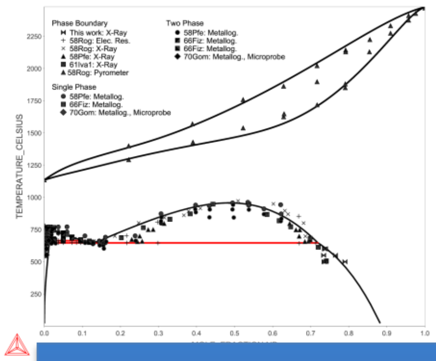
Multi-scale Modeling Example: Discontinuous Precipitation

Discontinuous Precipitation in U-Nb Alloys

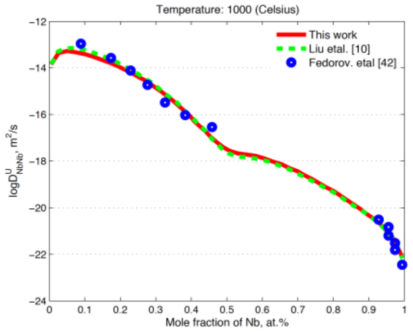
DFT



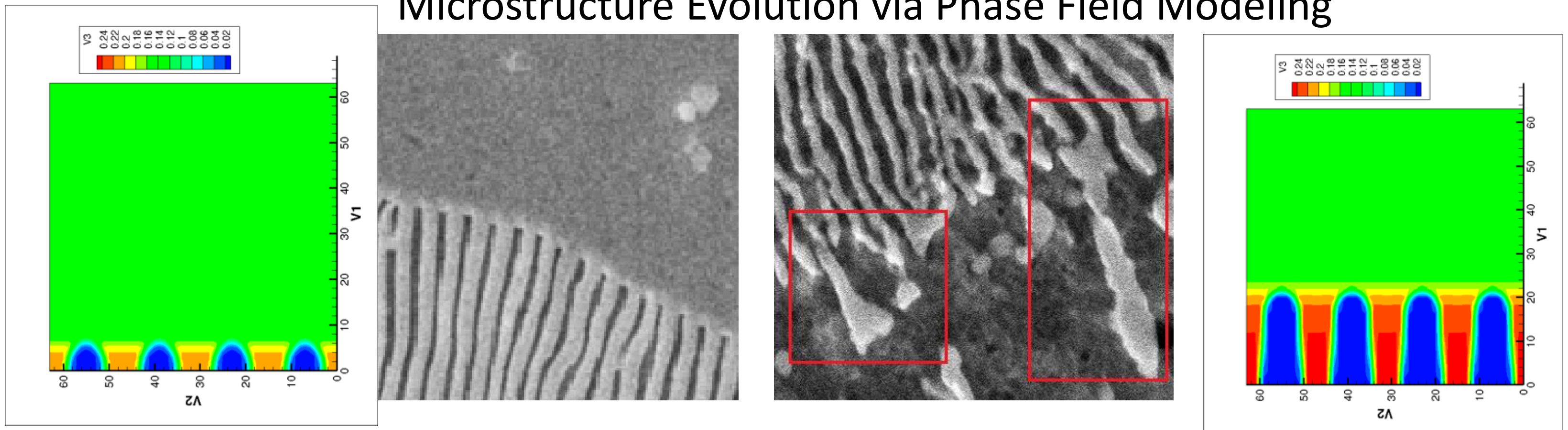
Phase Diagrams



Diffusivities



Microstructure Evolution via Phase Field Modeling



MATERIALS SCIENCE & ENGINEERING
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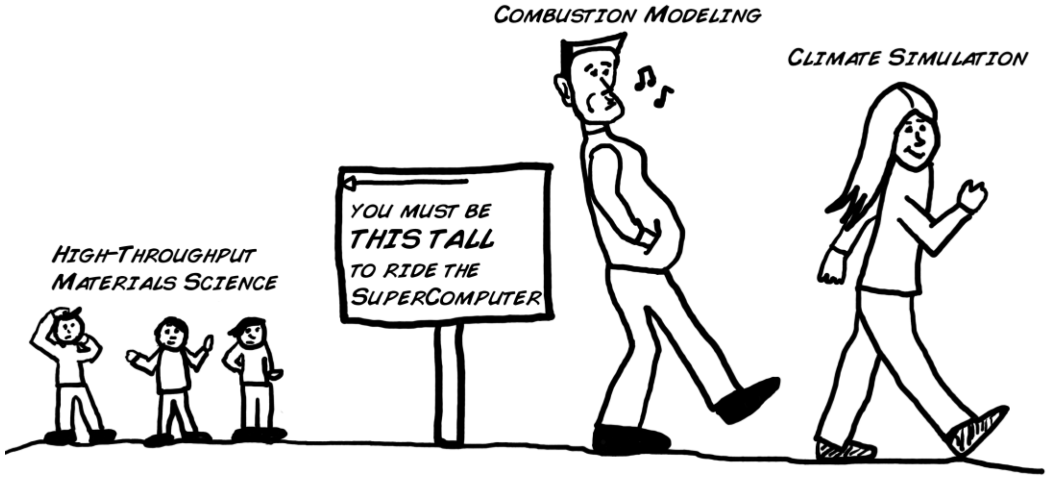
High-throughput DFT

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

High-Throughput DFT

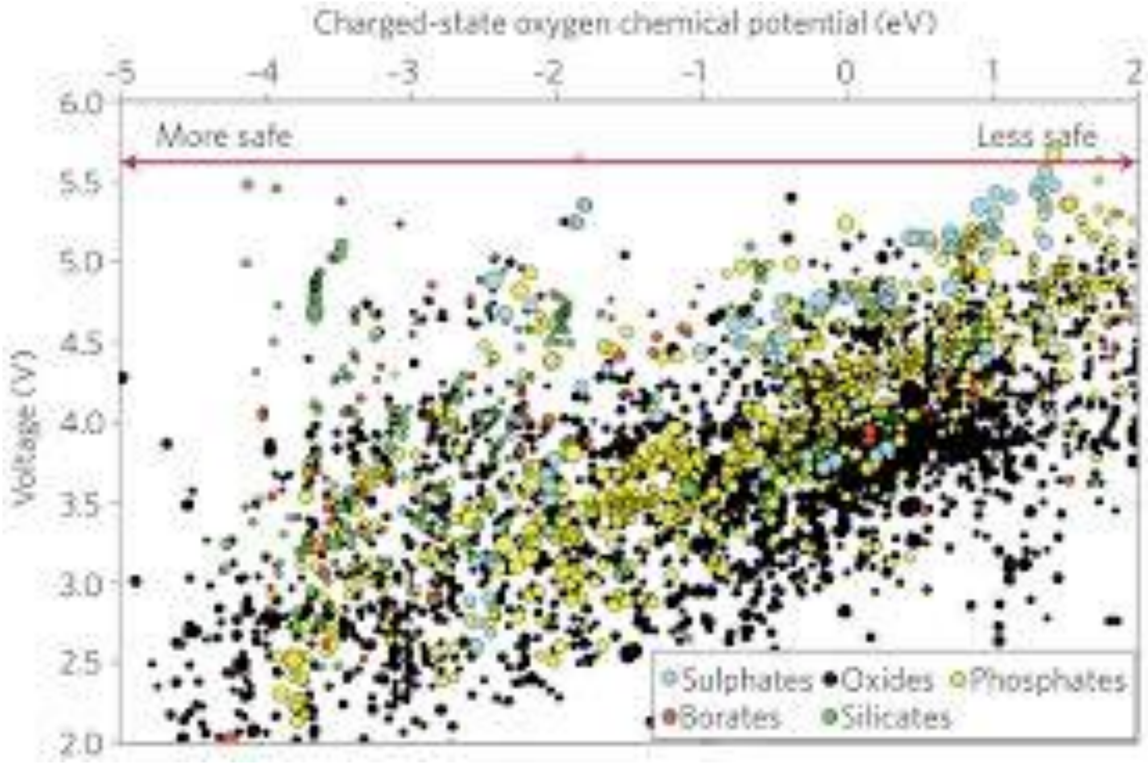
- DFT- First Principles Calculations
- High computational cost
- Increased computational resources make it possible to do 'high throughput' computational analysis
- Tool Development: TAMMAL



[Materials Project, MIT]

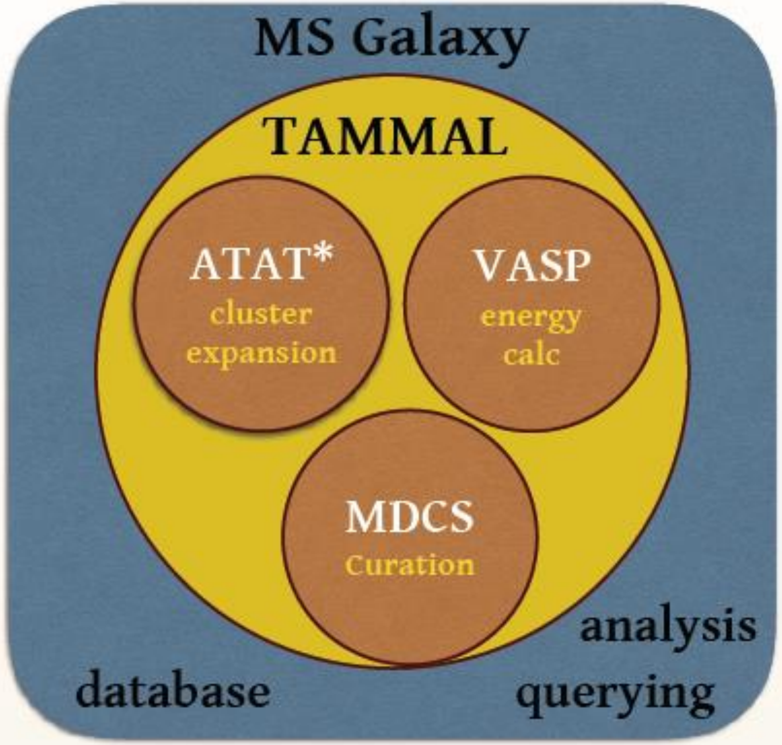
High-Throughput DFT

- Many (relatively small) problems
- Massively parallel computing tasks (e.g. high-throughput ab initio)
- Embarrassingly parallel simulations (e.g. Monte Carlo)



HT Engine: TAMMAL

- Use of **TAMMAL** (**Texas A&M Materials Automation Library**)
- Python-based suite of tools developed at TAMU Computational Materials Science Lab - Arroyave Group
- Automated means to control the entire workflow of computational research
- Design complex computational workflows
- Integrate with the Materials Data Curation System (MDCS) developed at NIST
- Generates and maintains a materials database within MS-Galaxy
- Design complex analysis workflows



TAMMAL enables high-throughout calculations for hundred of systems while allowing for complex workflows

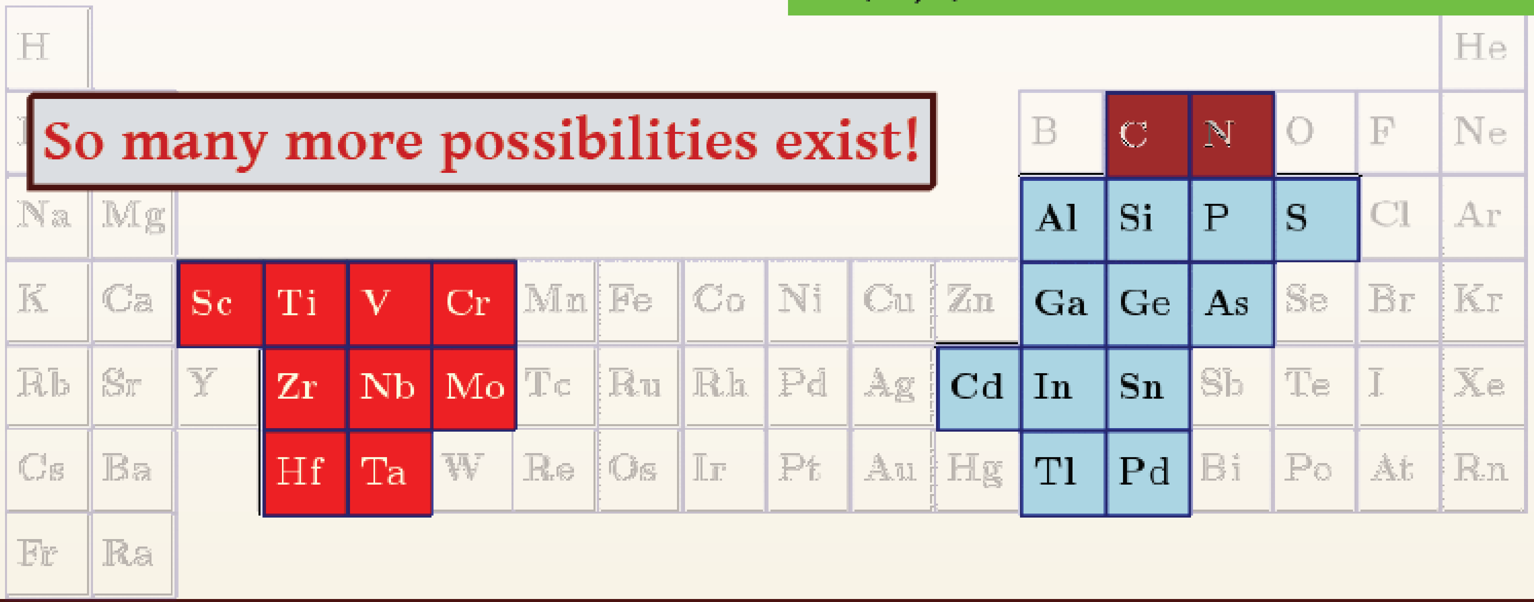
Alloy Theoretical Automated Toolkit (ATAT) (*[2002] A. Van de Walle et al.*

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Example: MAX Phases

- Novel class of layered inter-metallic compounds with unique properties
- 792 possible MAX phases
- Even larger set of possible solution MAX phases

- Some known 211 solid-solution (M-site) MAX phase systems include:
- $(Ti,V)_2AlC$, $(Ti,Nb)_2AlC$, $(Ti,Cr)_2AlC$, $(Ti,Ta)_2AlC$
- $(Ti,Hf)_2InC$, $(Ti,Hf)_2InC_{1.26}$, $(Ti,V)_2SC$
- $(V,Nb)_2AlC$, $(V,Ta)_2AlC$, $(V,Cr)_2AlC$,
- $(Nb,Zr)_2AlC$
- $(Cr,V)_2GeC$



Raymundo Arróyave
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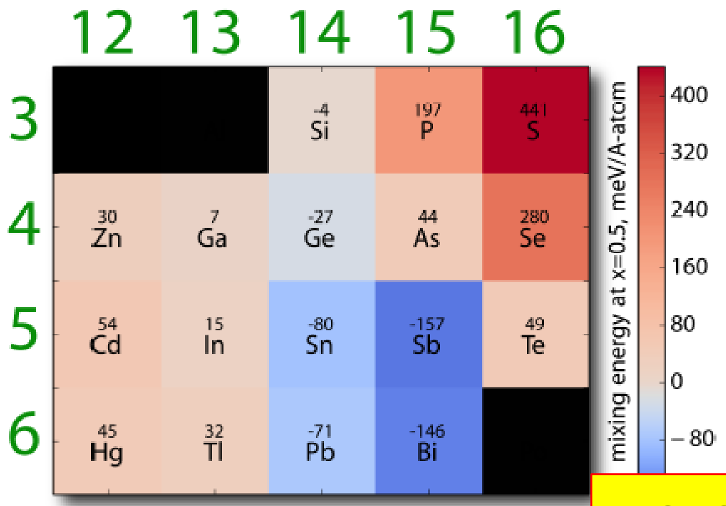
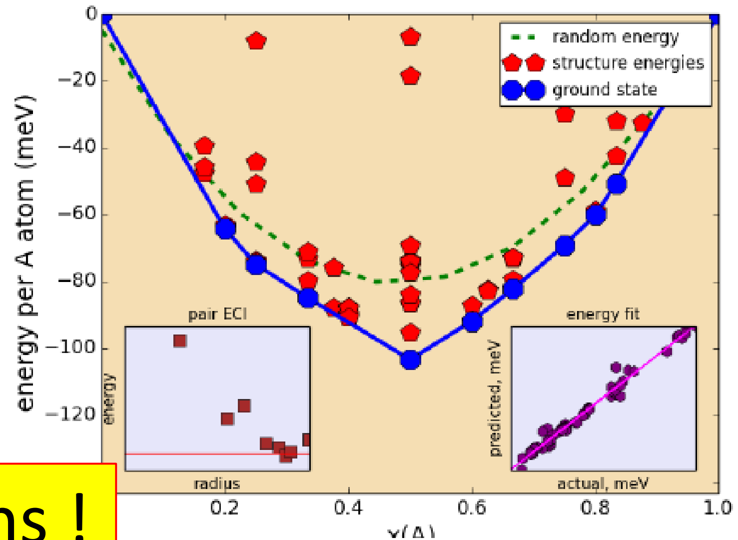
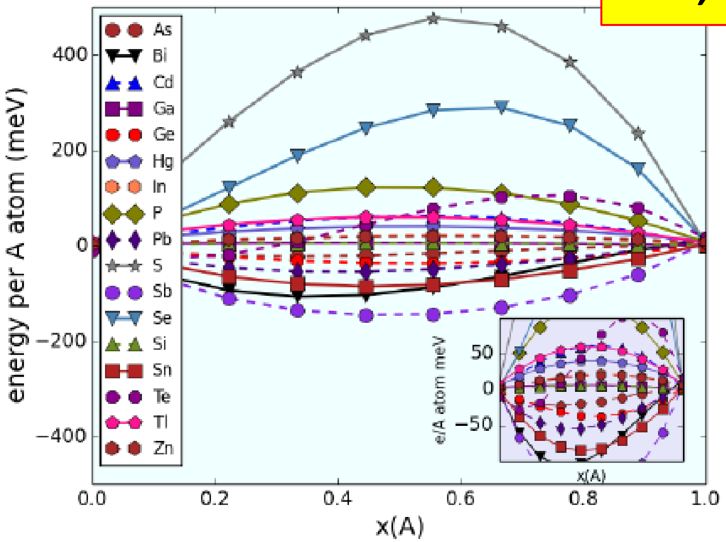
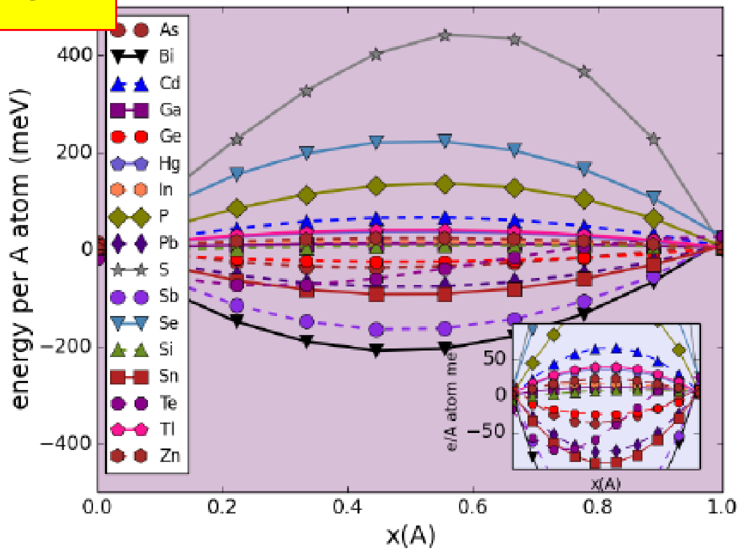
Example: MAX Phases





10,000’s calculations !





Materials Modeling as a Tool for Design

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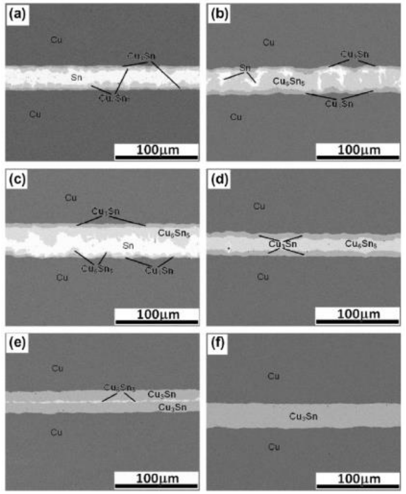
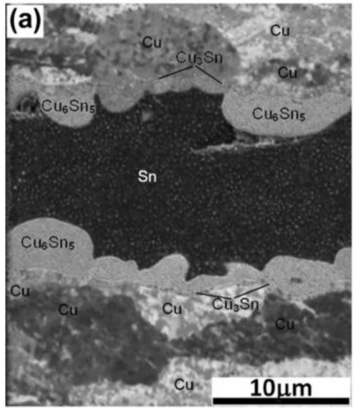
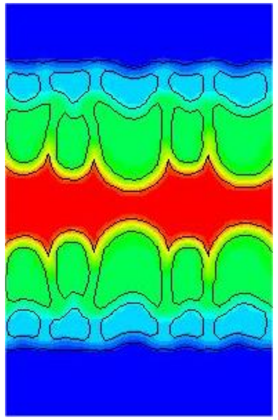
Extrapolation to other Geometries

1. Elimination of Cu and Cu6Sn5

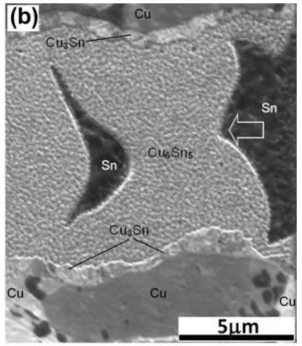


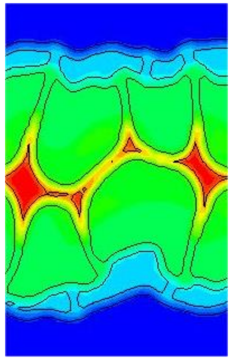
2. Scallop-like morphology (Cu6Sn5)



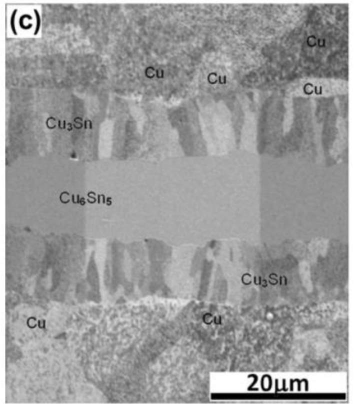


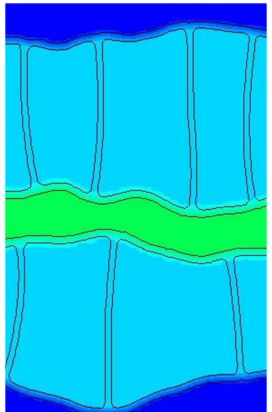
3. Isolated "lakes" of Sn and Thickness ratio of Cu6Sn5 and Cu3Sn





4. Column-like morphology of Cu3Sn

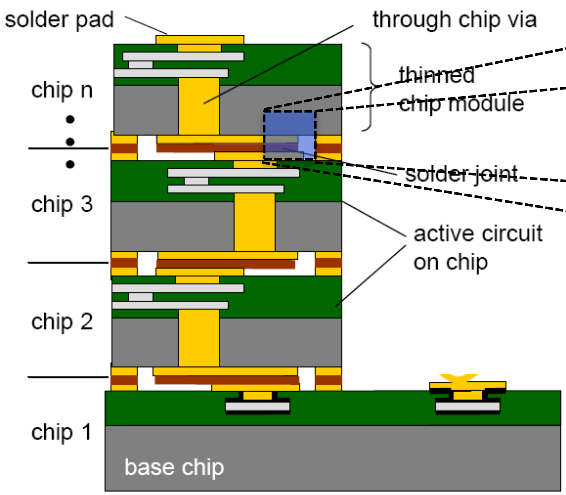




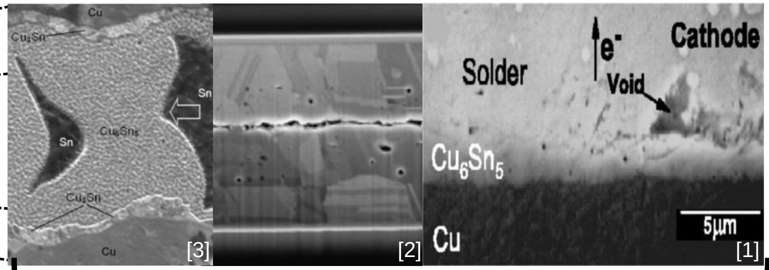
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Simulation-Assisted Interconnect Design

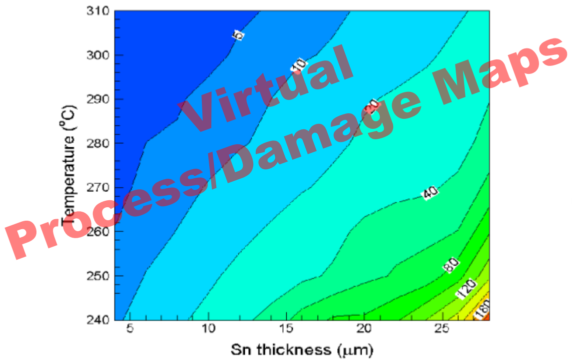
Packaging Application



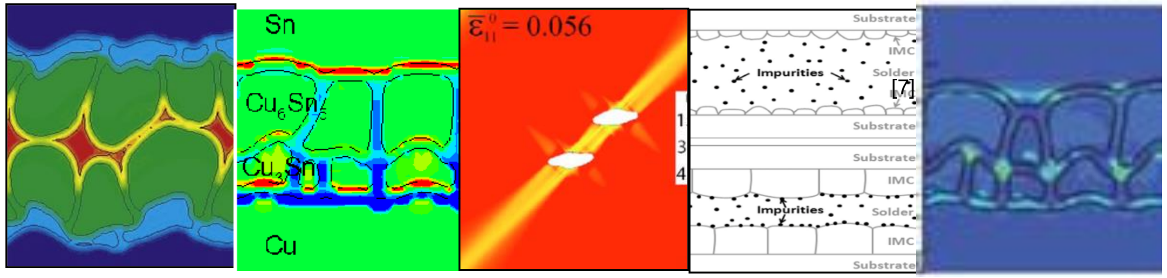
Interconnect Formation/Evolution



Computational Investigation
Multi-Physics Phase Field Modeling

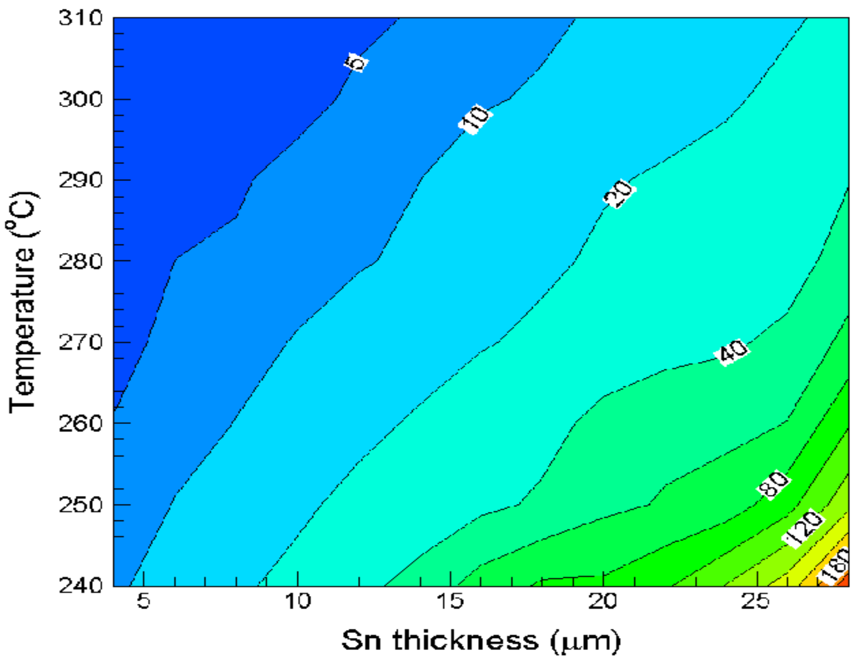


IMC Impingement | Electromigration | Microelasticity | Segregation | Void Formation

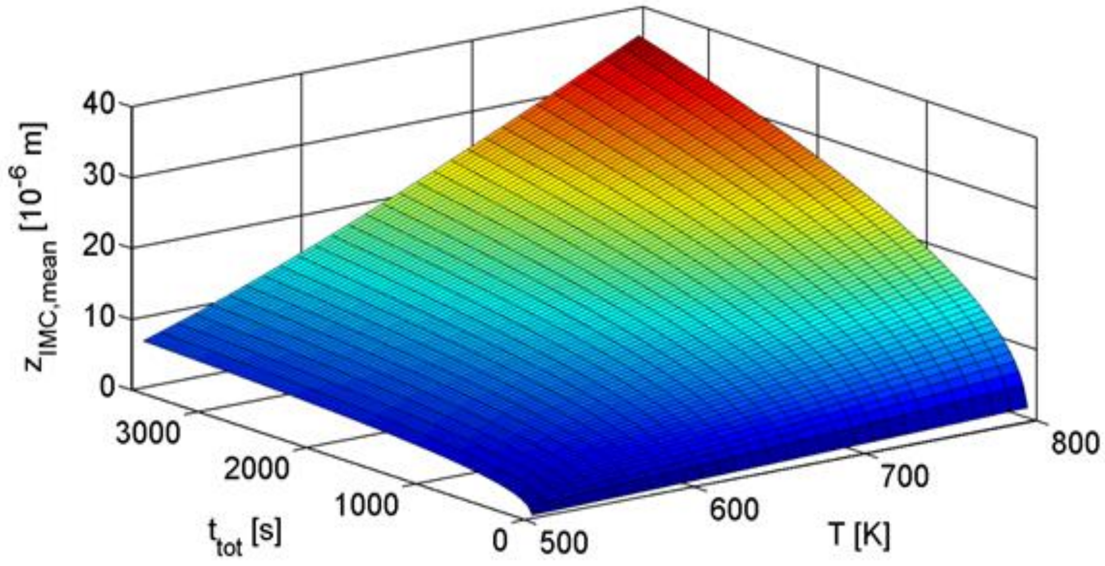


Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Simulation-Driven Process/Damage Maps



Cu-Sn TLP [Park 2014]



Ag-Sn TLP [Lis 2014]

(solidification time)

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

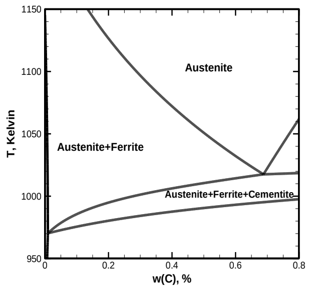
Connecting Alloying/Processing-Microstructure-Properties

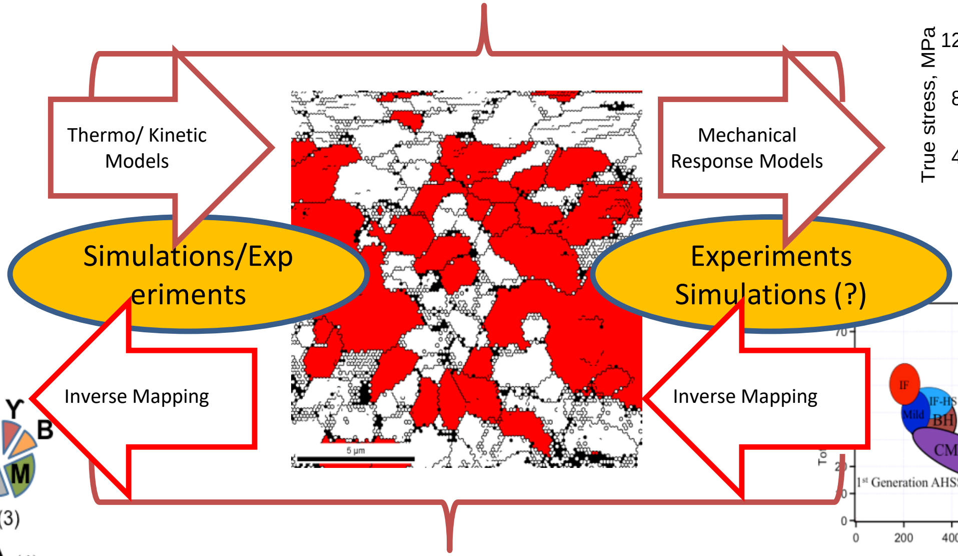
Inputs:
Composition, Heat Treatment, Thermo-Mechanical Processing

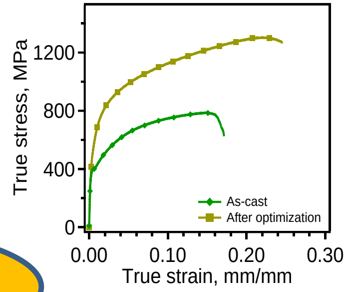
Attributes
Phase Constitution
Microstructure

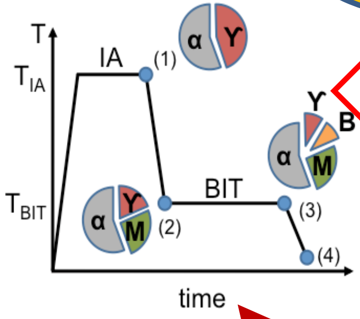
Performance
Strength
Ductility

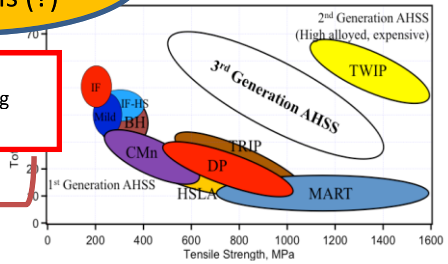
Analysis/Discovery







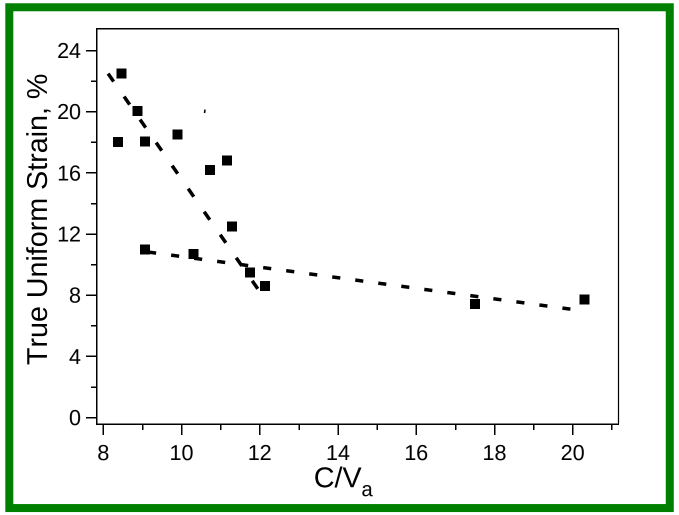


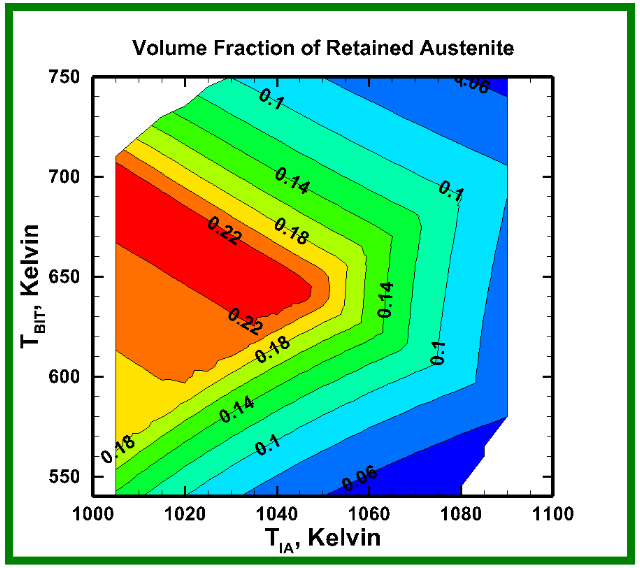


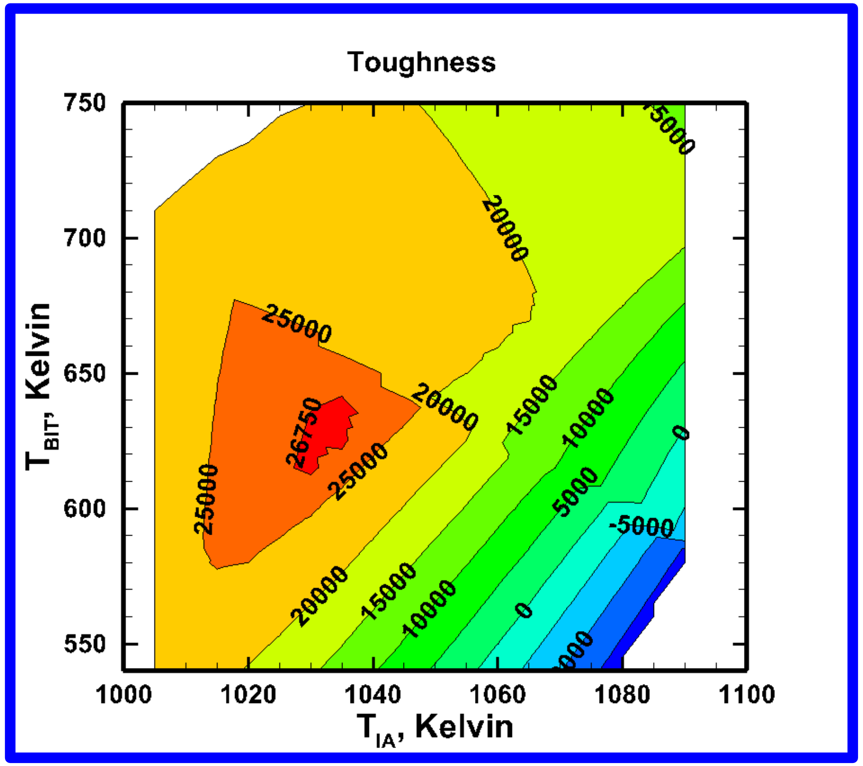
Synthesis/Design

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Putting Everything Together: Synergies between Experiments + Simulations

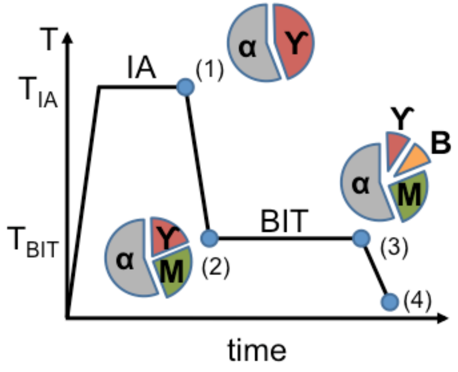




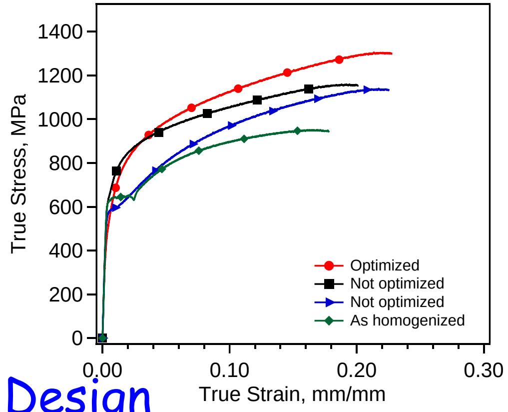


Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

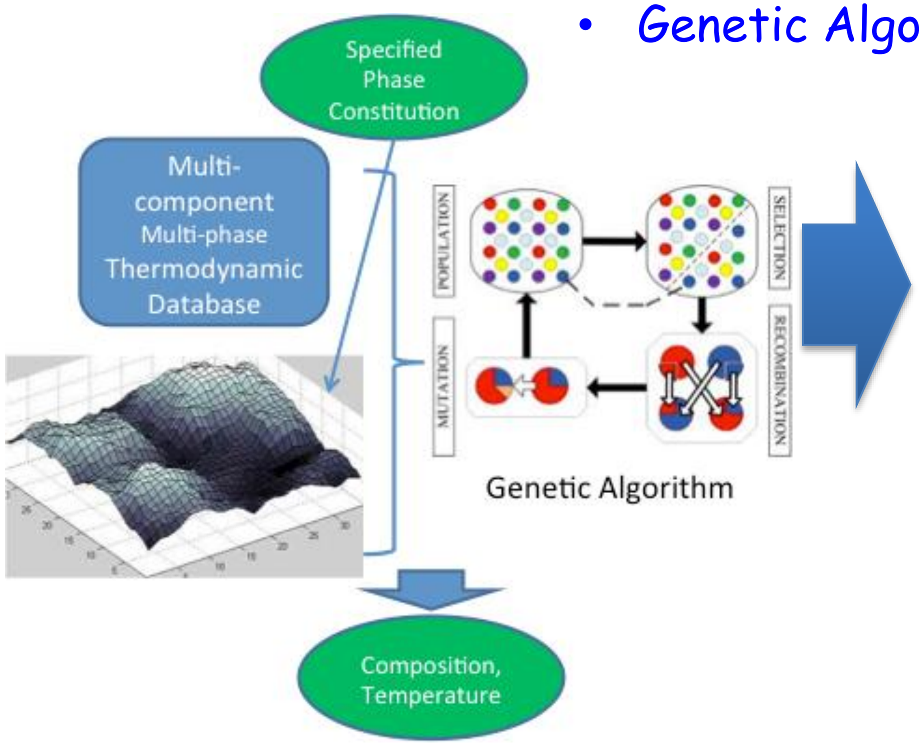
A New Framework for Materials Design:

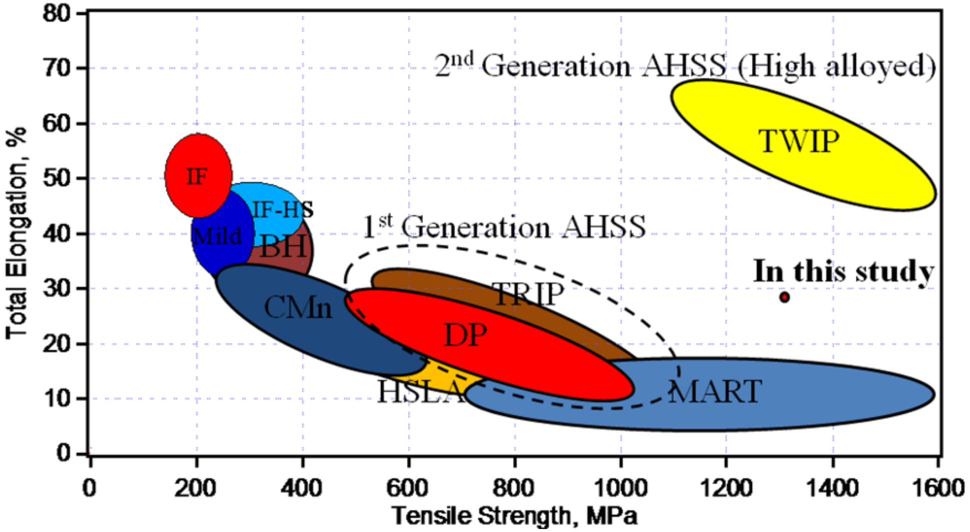


- Heat Treatment Design

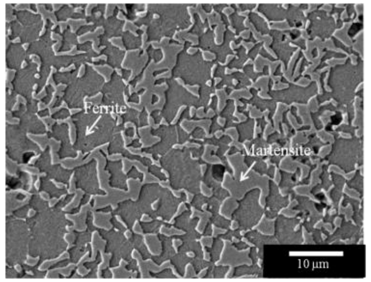


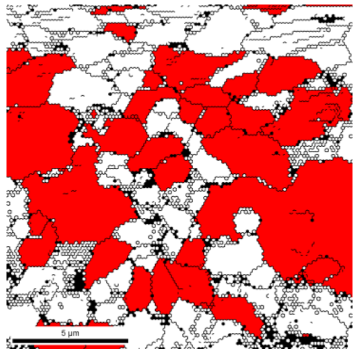
- Genetic Algorithm-based Alloy Design





- Experimental Characterization

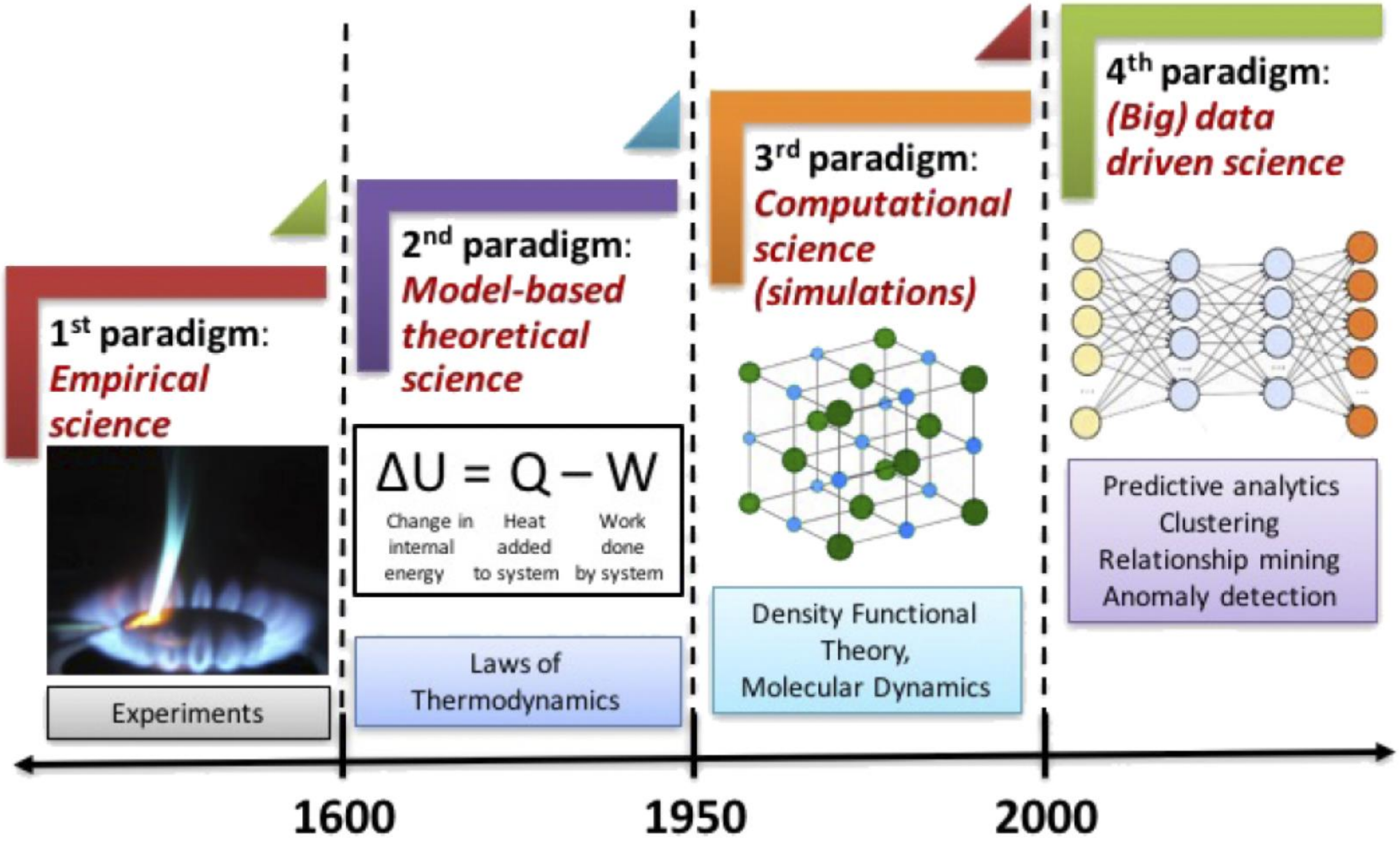




Materials Informatics

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

The Fourth Paradigm:

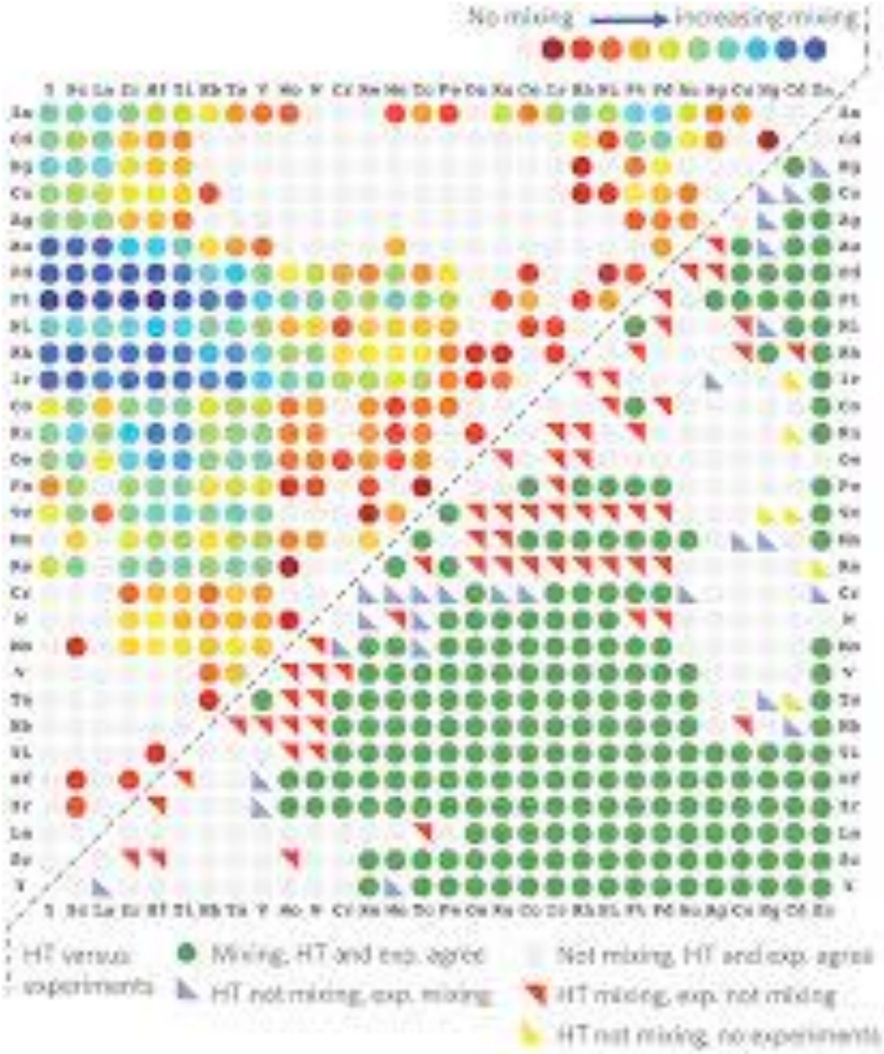


2016 Agrawal (APL)

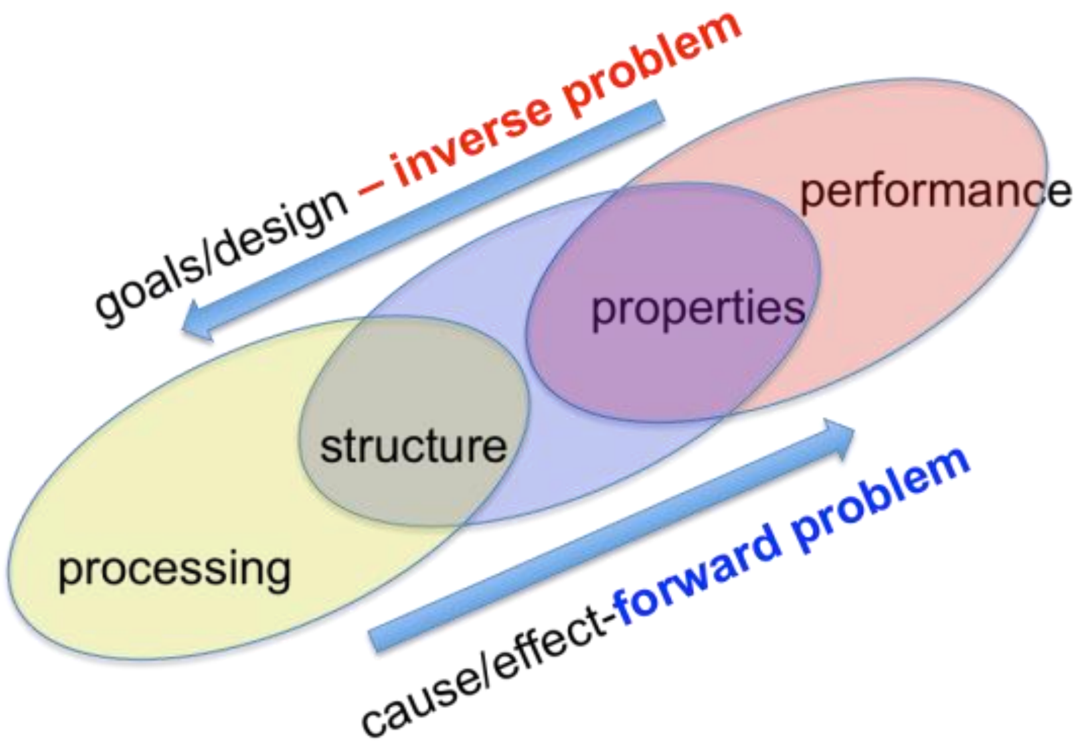
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University
MATERIALS SCIENCE & ENGINEERING TEXAS A&M UNIVERSITY

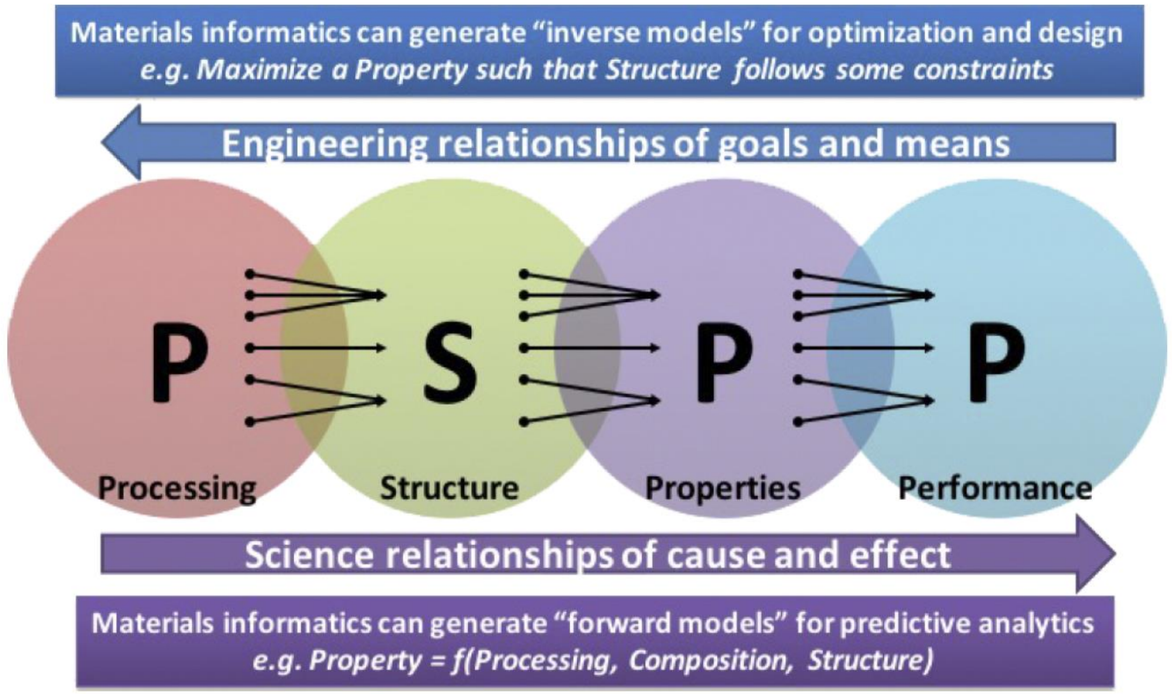
Materials Informatics

- Identify correlations between materials descriptors and performance indicators
- Correlations between multi-dimensional data points
- Use sophisticated informatics approaches (i.e. classification/regression)



Connections Along Materials Science Paradigm





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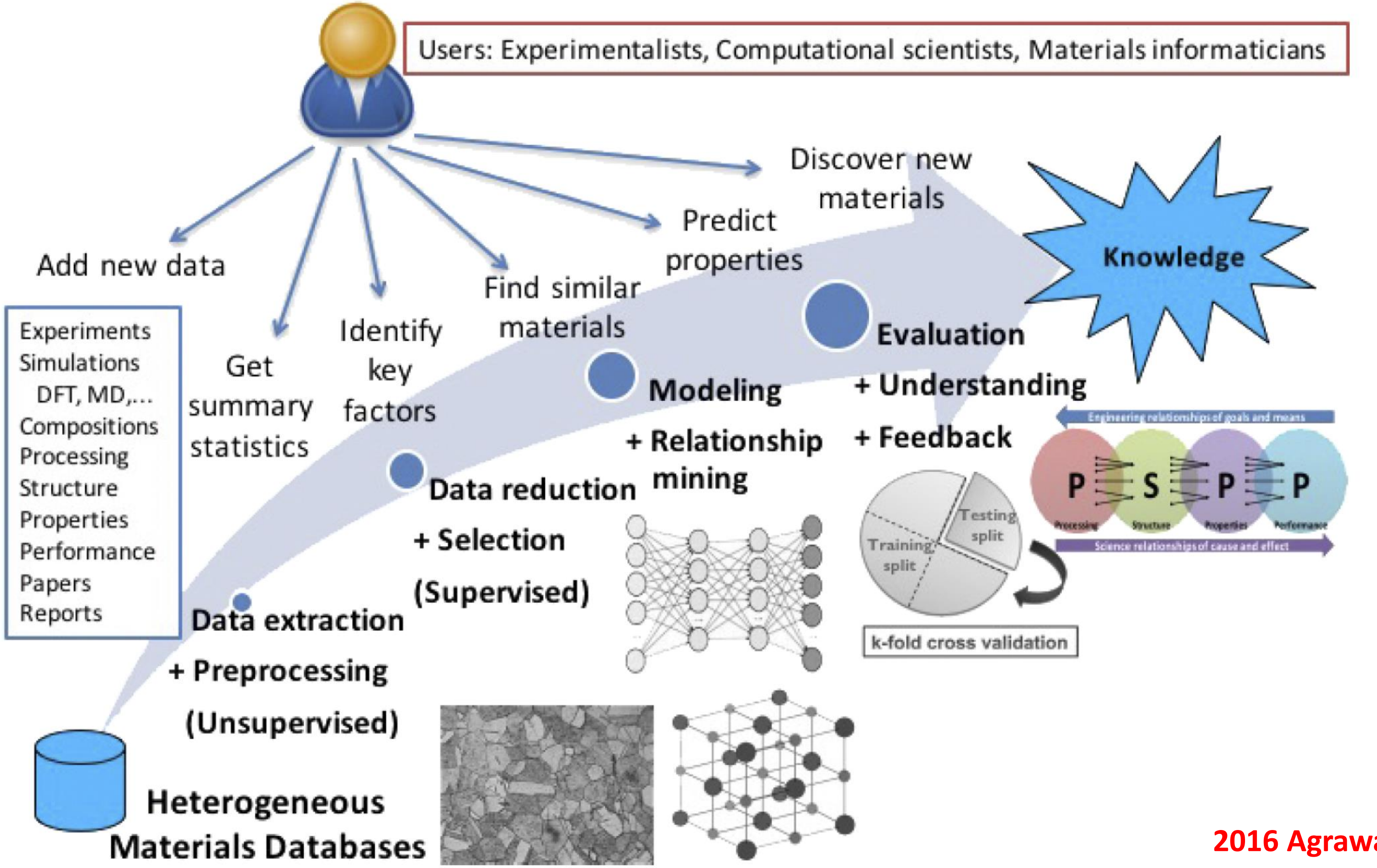
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Data-Enabled Materials Discovery



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Accelerated Development of Materials, The Future Is Here (!)

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

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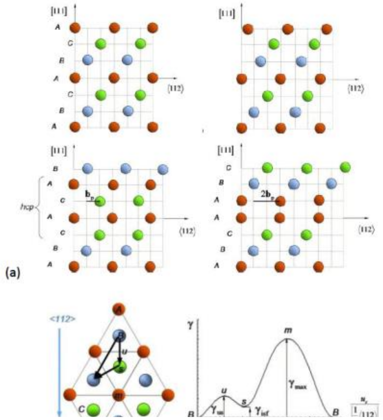
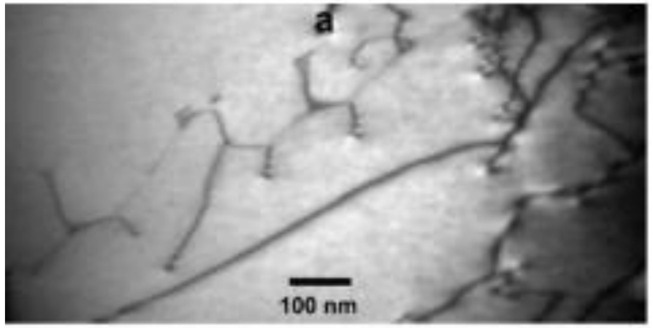
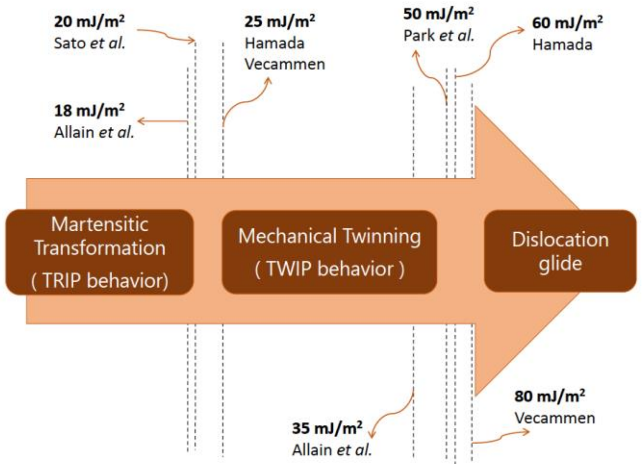
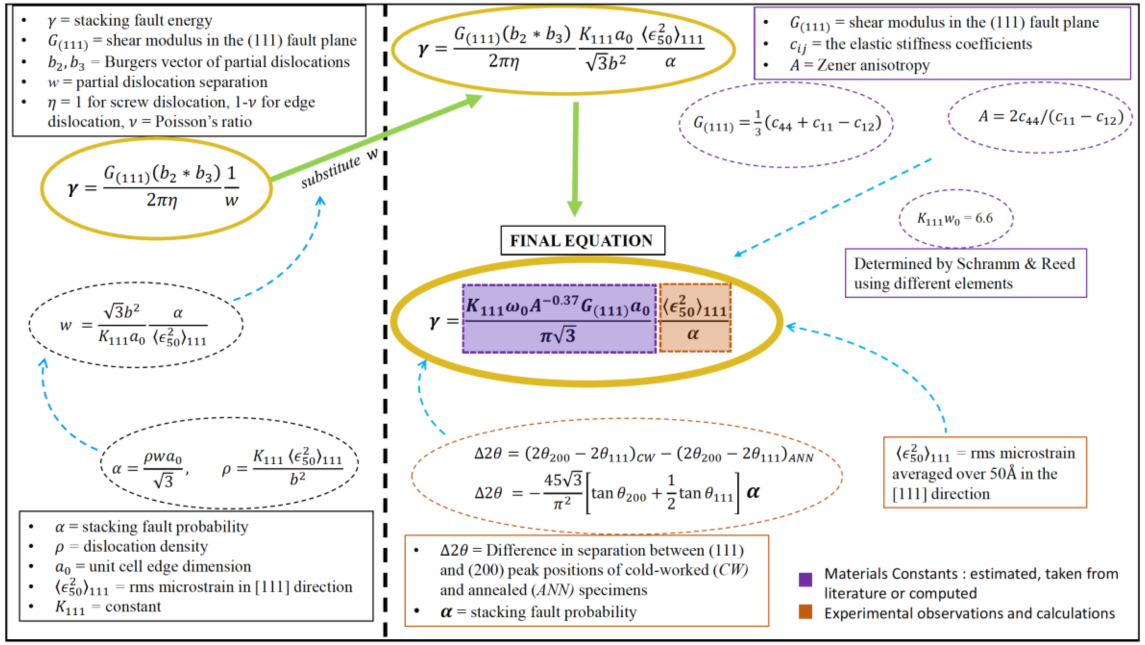
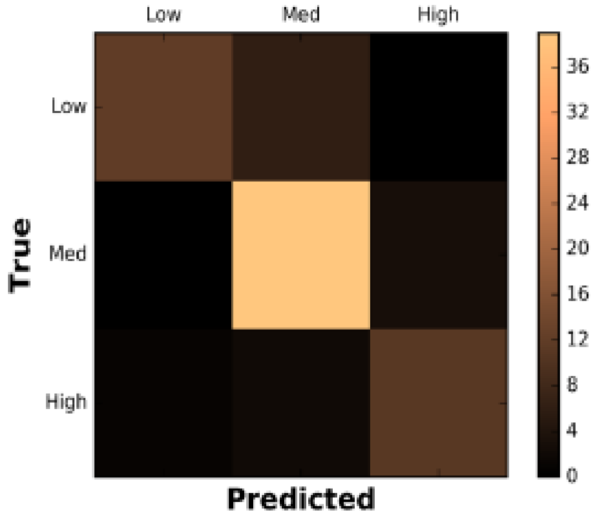
Materials Informatics in my Group









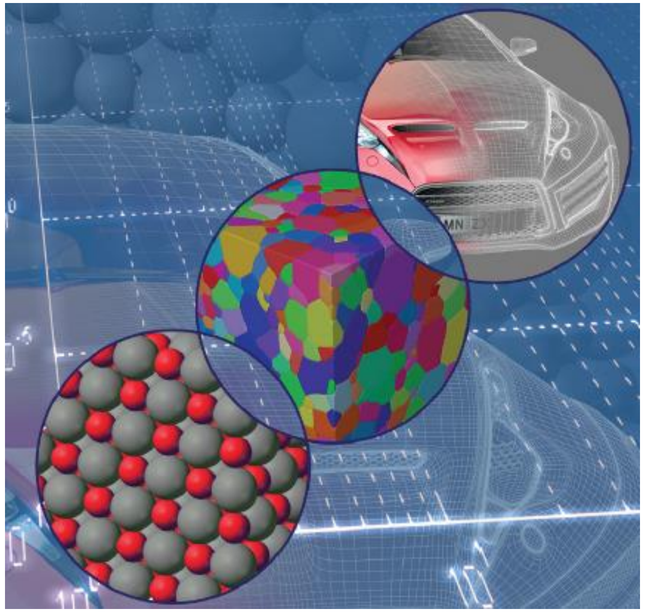


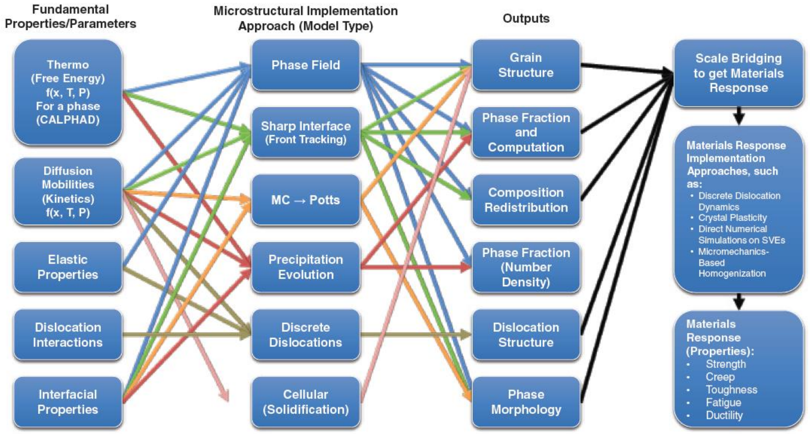
Current Challenges

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Computational Materials Science

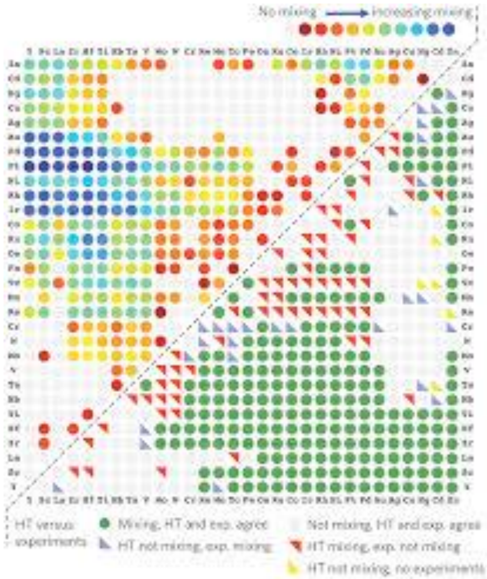
- Multi-scale problem must be explicitly tackled.
  - Some progress in length-scale bridging. Not much on bridging time scales
  - No unified code. Need to create interfaces among multiple codes
  - Full multi-scale approach is still incredibly expensive

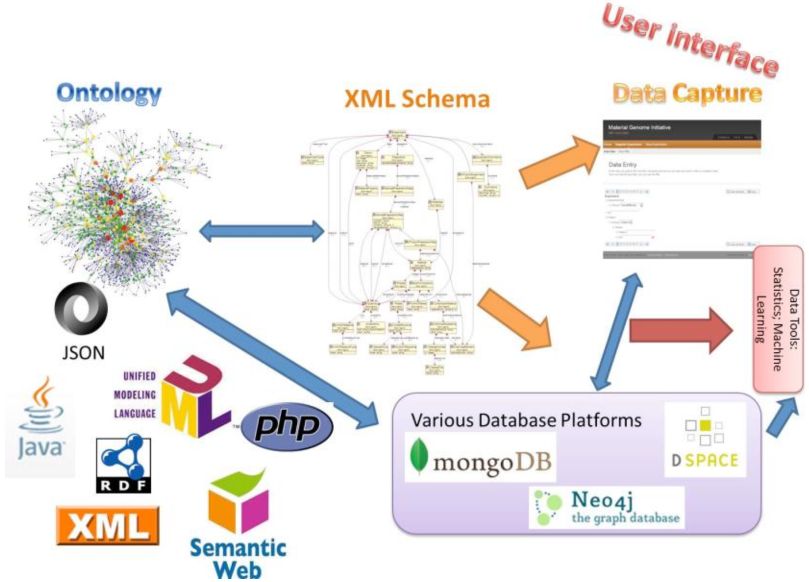




Materials Informatics

- Materials Science's Big Data Flavor is mostly of the 'Variety' Kind
- Do not have (yet) materials informatics infrastructure.
- Materials data is scarce and difficult to come by.
- It is not clear that 'data' on its own is sufficient. There is no free lunch

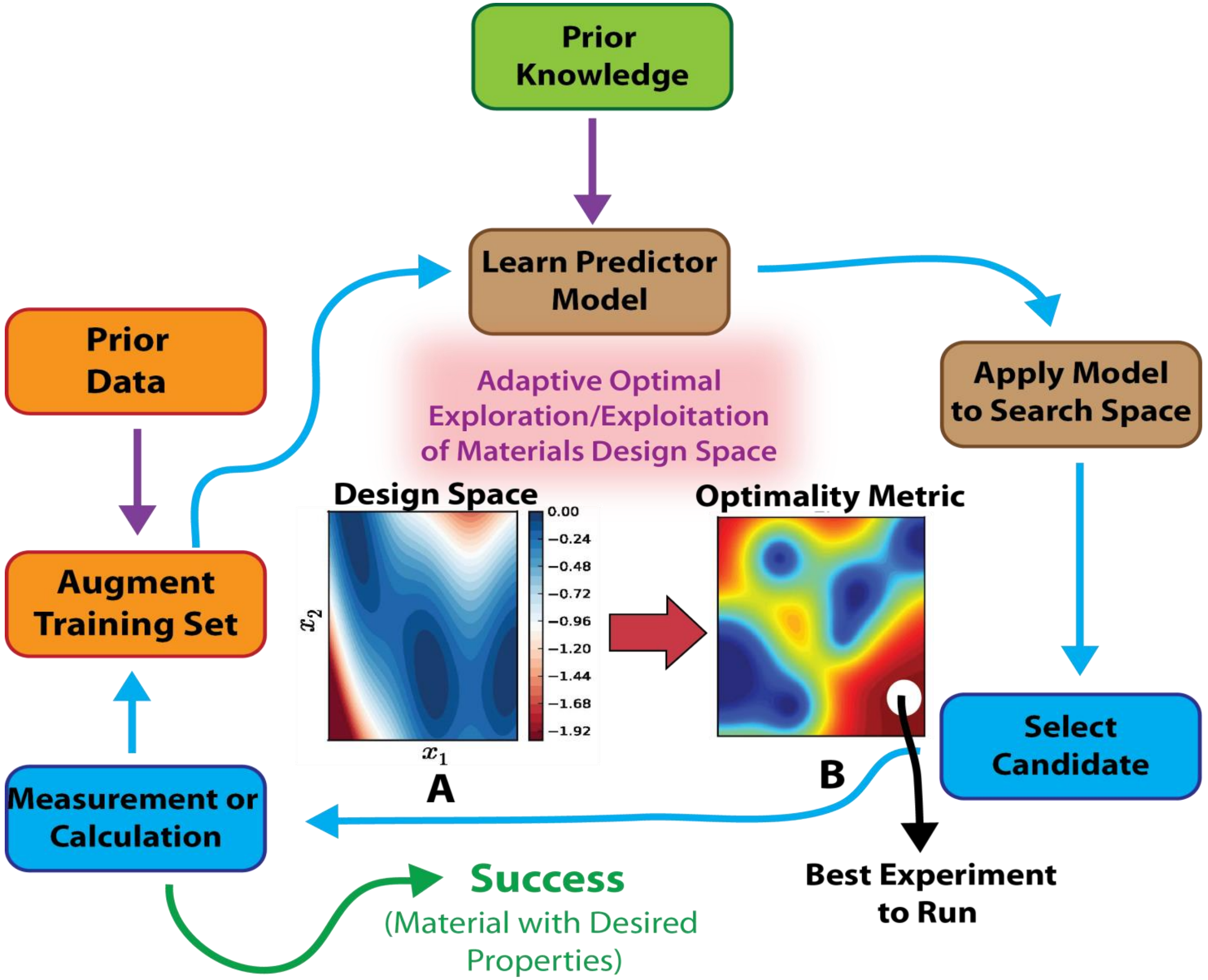




Beyond Computer-Aided Materials Design

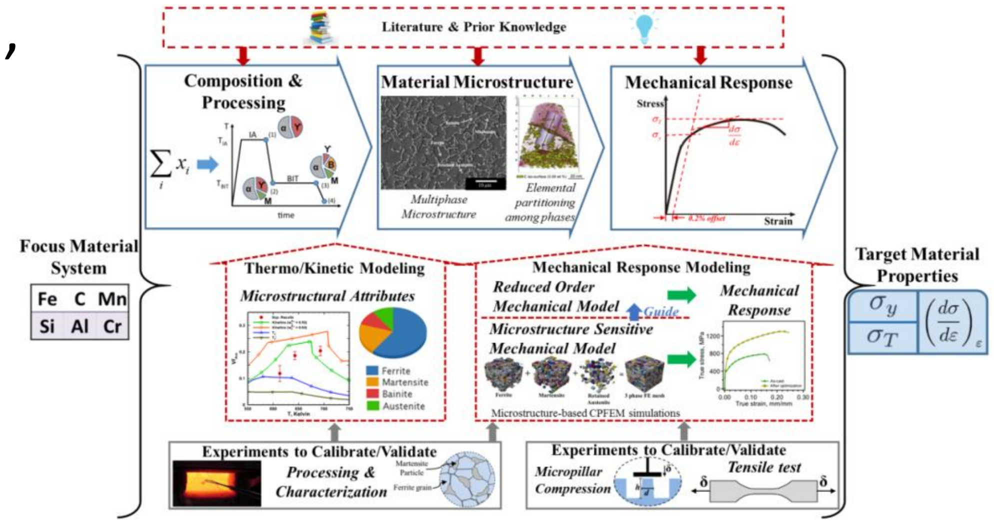
Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

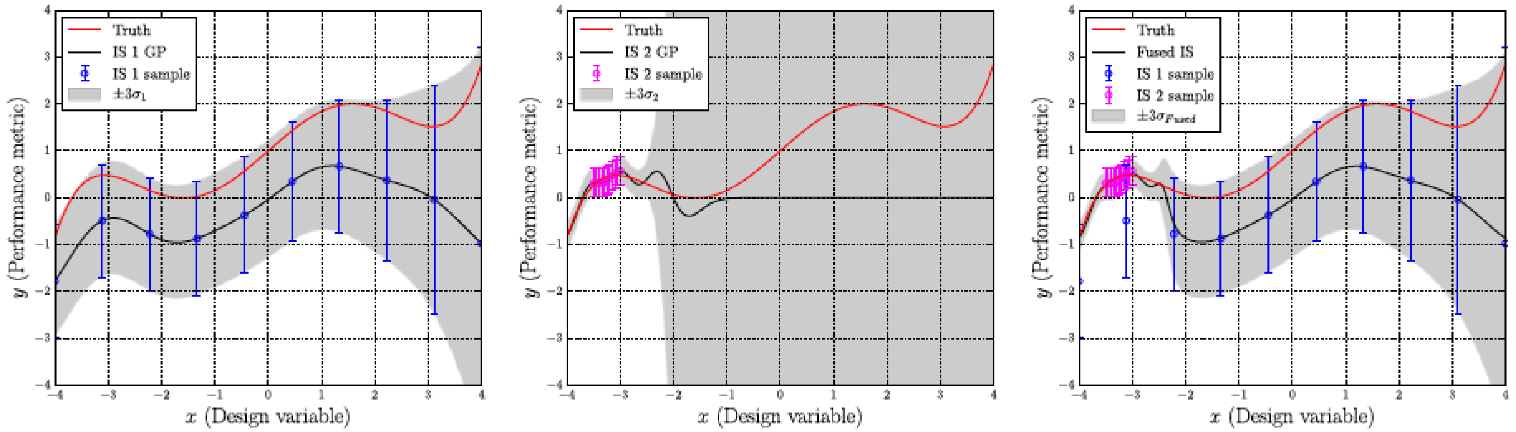
Adaptive Materials Discovery



Source-Agnostic Materials Discovery

- Forget about ‘experiments’, ’computations’ and ‘data’
- Everything is essentially an ‘information source’
- There may be ways of fusing information that exploits strengths of different ways of learning about materials while minimizing weaknesses
- This is still completely unexplored





Thanks to: D. Allaire and A. Srivastava

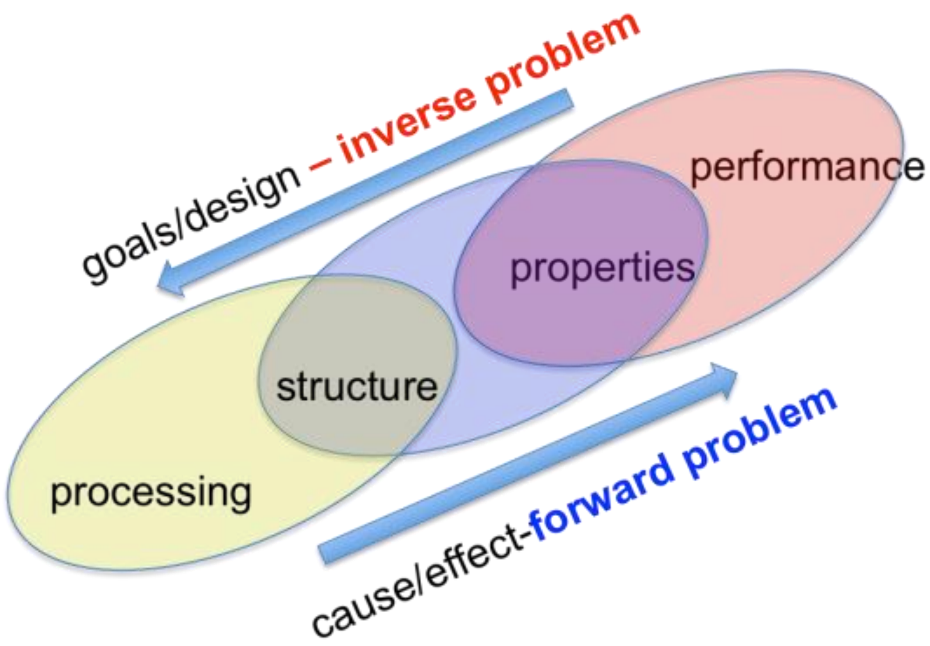
Fusing Multiple Sources Together

Source 1: Expensive Multi-scale Model

Source 2: Cheap Effective Model

Source 3: Statistical Model

Source 4: Theory



HOW?????

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Conclusions

Raymundo Arróyave
Department of Materials Science and Engineering, Texas A&M University

Conclusions

- Materials Development is a Hard Problem
- Recent advances in computational resources (hardware/software) have made computer-aided materials development possible
- Recent emphasis on data-driven materials development promises even more dramatic advances
- There are limitations in these approaches, that can be alleviated if we instead go source-agnostic