Tools For Materials Design

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CHiMaD

TOOLS

- Goal: Integrate computations and databases in the materials design process
- To accomplish this new tools are needed:
  - Theoretically Informed Coarse Graining and Evolutionary Design
  - Microstructure Development
  - Rapid Throughput and High Resolution Characterization
  - Integration – Accelerated Insertion of Materials

Microstructure Development

- Objective: Model the microstructural evolution of multiphase multicomponent materials
- Phase field methods
  - Easy to add new physics
  - Allows for topological singularities
  - No need to track phase boundaries explicitly
- Level Set
  - Allows for topological singularities
  - No need to track phase boundaries explicitly

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Phase Field

- Develop a community code
- One of the closest is FiPy
- Example: nanowire growth, captures fluid dynamics capillarity and diffusion
- Goals:
  - Allow for the incorporation of CALPHAD databases
  - Port to leadership class machines (ANL)
  - Preconditioners/PETSc (ANL)

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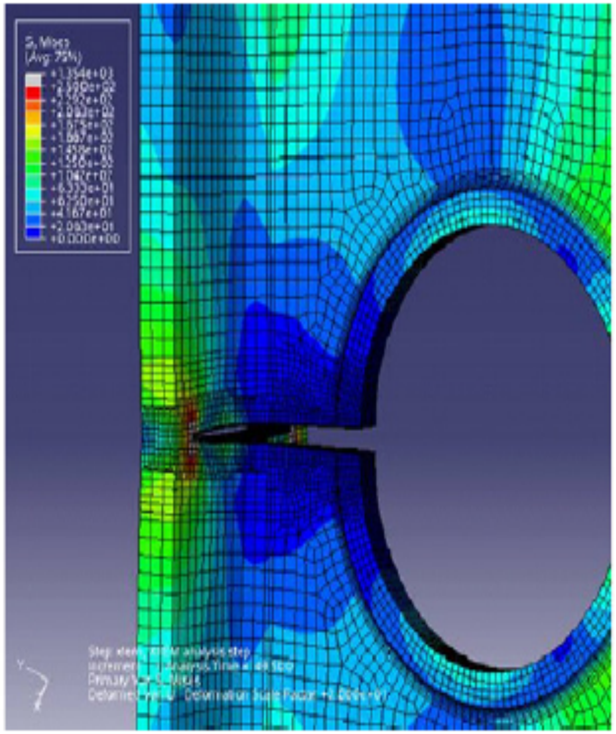
Schwalbach, Davis, Voorhees, Warren and Wheeler

Level Set

- Many of the advantages of the phase field method
- Does not employ a diffuse interface
- May be easier to integrate with CALPHAD databases



Shi, Liu and Chopp

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Rapid Throughput and High Resolution Characterization

- Goal: provide the data to populate the databases needed for the use-case groups
- This can be done using calculations and experiments
- Calculations: Wolverton group's Open Quantum Materials Database
  - Over 300,000 compounds, and counting
- Experiments:
  - Co-sputtering using three or more pure sources
  - Diffusion between blocks of two or more pure materials
  - Challenge: methods for rapid characterization

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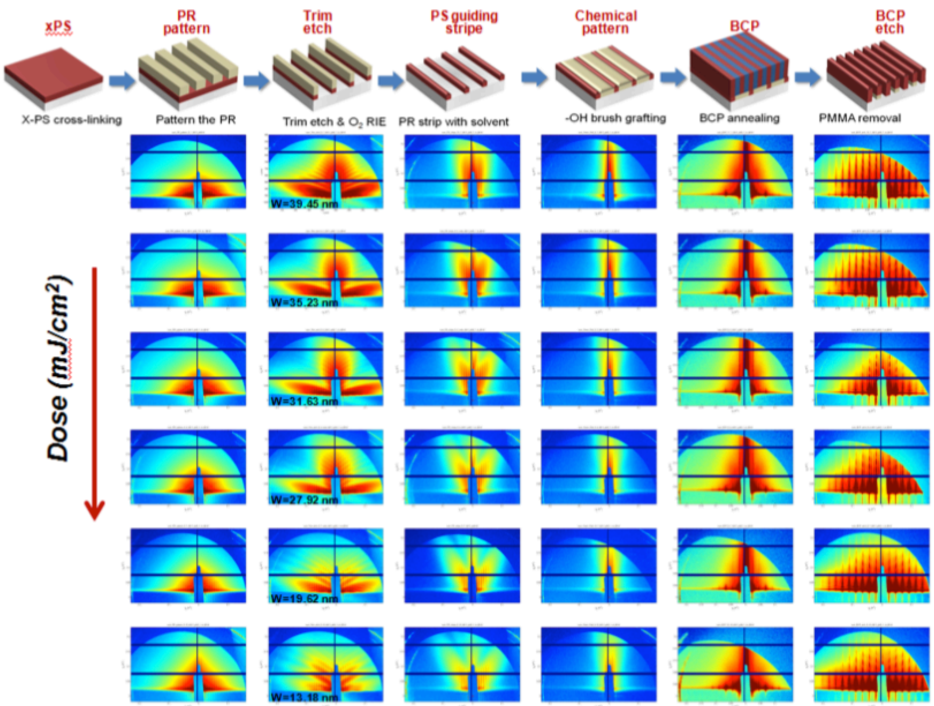
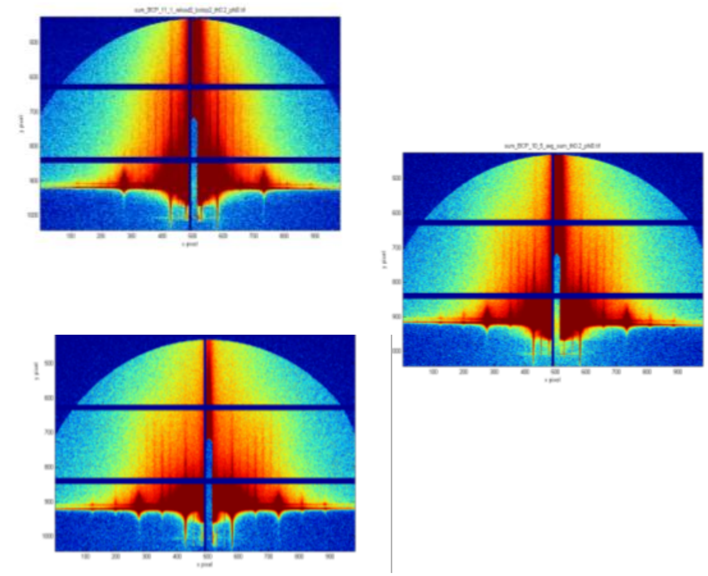
Vision of Integrated Analysis Loop: towards a forward model

GISAXS data

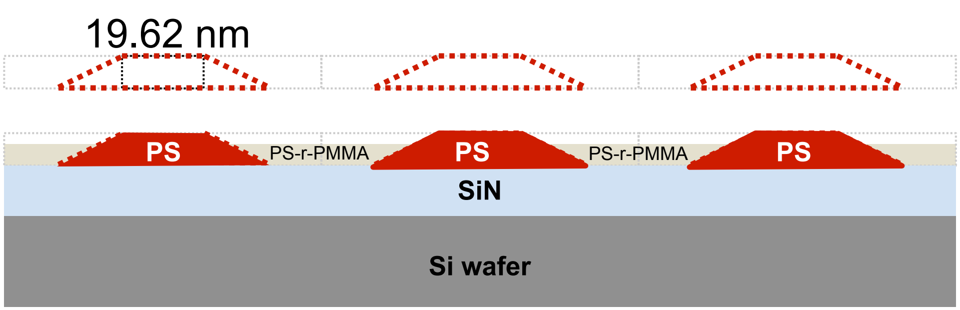


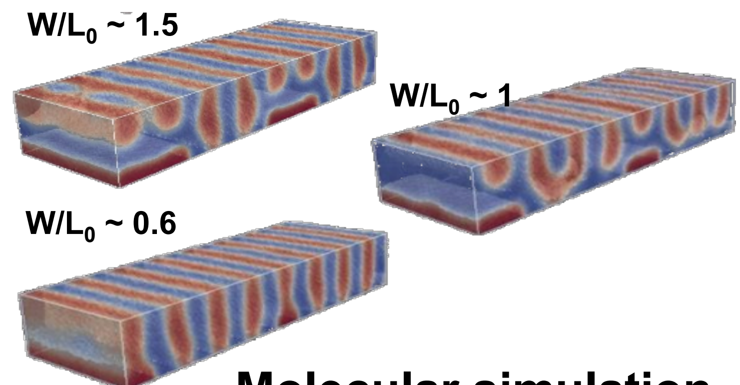
GISAXS from BCP



Form factor and structural factor to generate GISAXS pattern

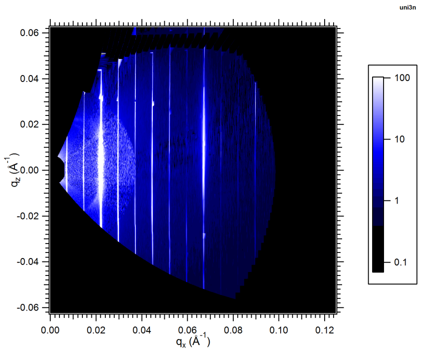
Boundary conditions for DSA

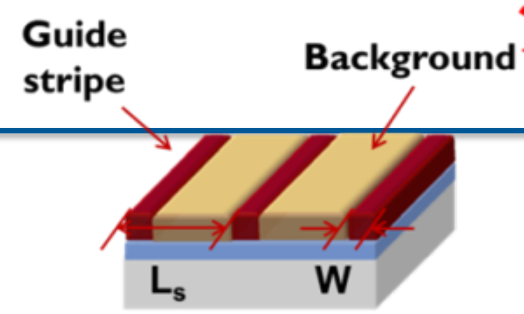




Molecular simulation

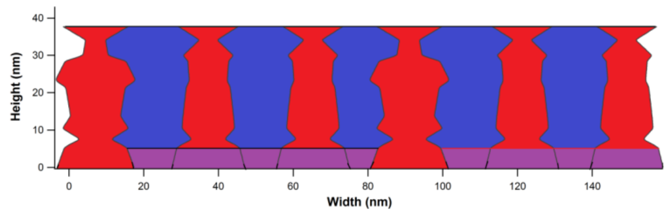
Experimental Results Compared to Simulations

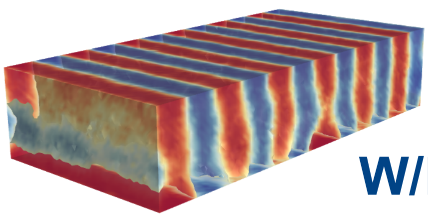




Geometry

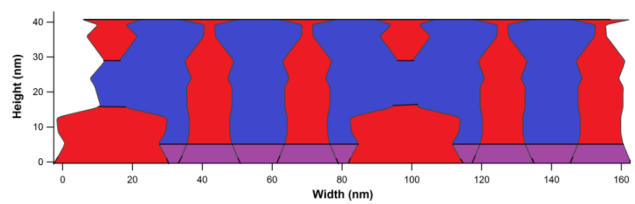
N11-6 $W/L_o = 0.75$

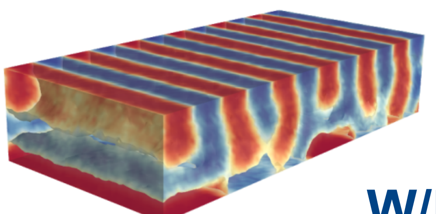




$W/L_o = 0.6$

N11_4 $W/L_o = 0.95$

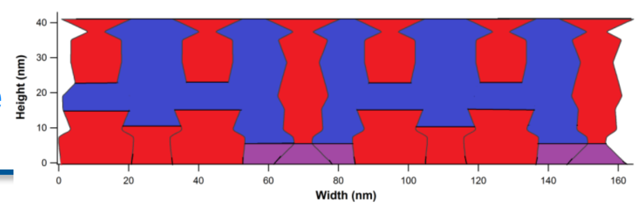


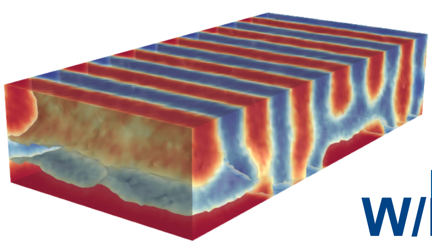


$W/L_o = 1.0$

N11-0 $W/L_o = 1.7$

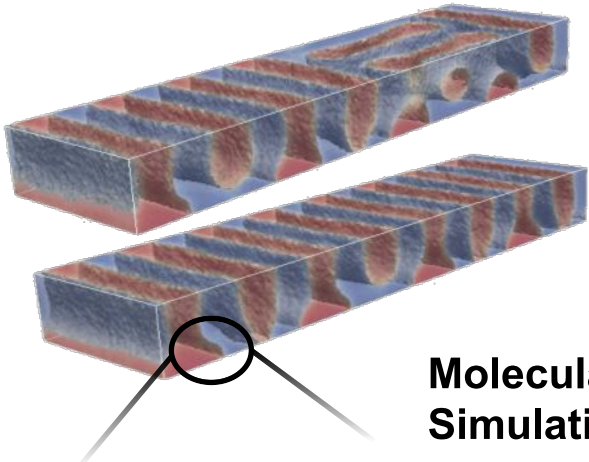
Nealey, De Pablo, Kline

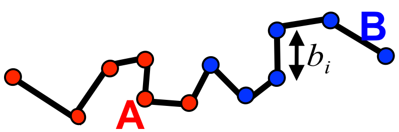




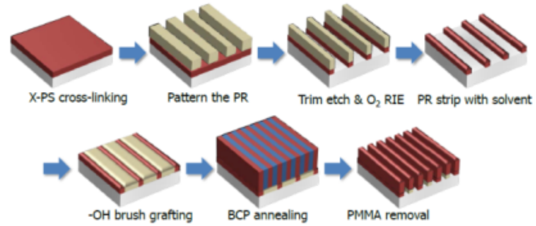
$W/L_o = 1.5$

Leveraged Resources for 3D Characterization of DSA at ANL



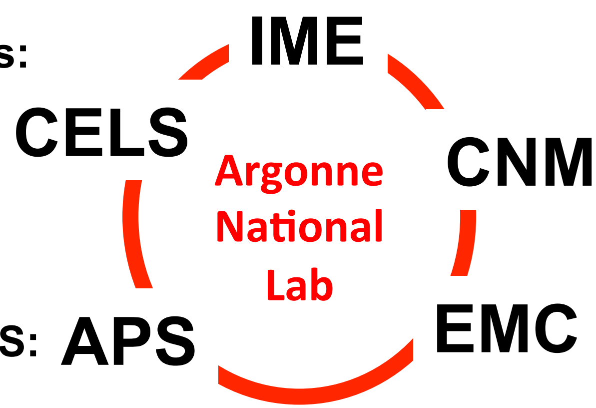


Molecular Simulations:



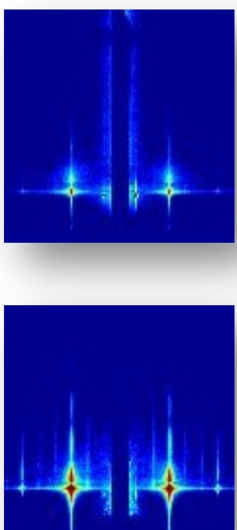
IME - Directed Assembly:

CNM – Nanofabrication:



- Electron Beam Lithography System
- RIE Oxford PlasmaLab 100
- Atomic Layer Deposition

EMC - TEM tomography:

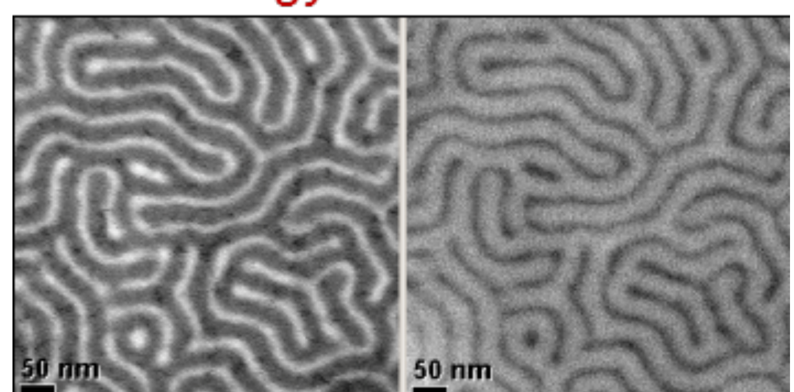


APS - GI-SAXS:

RoSXS

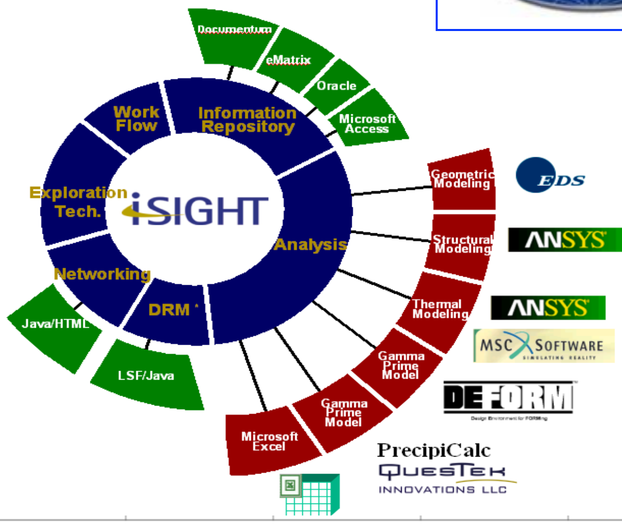
Sector 8, GISAXS, Sector 29, RSoXS

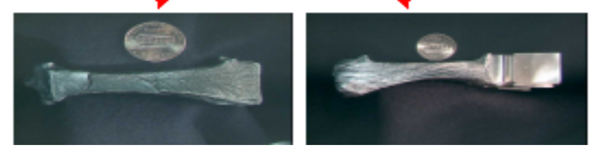
Energy-filtered TEM

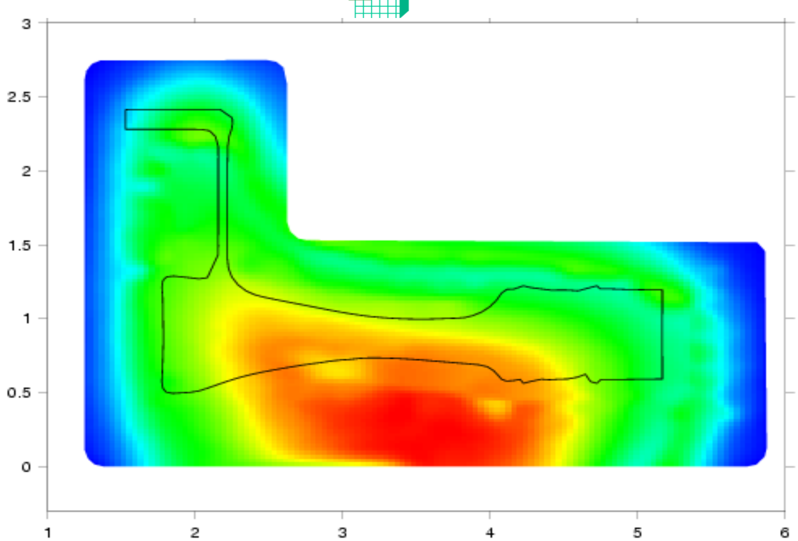


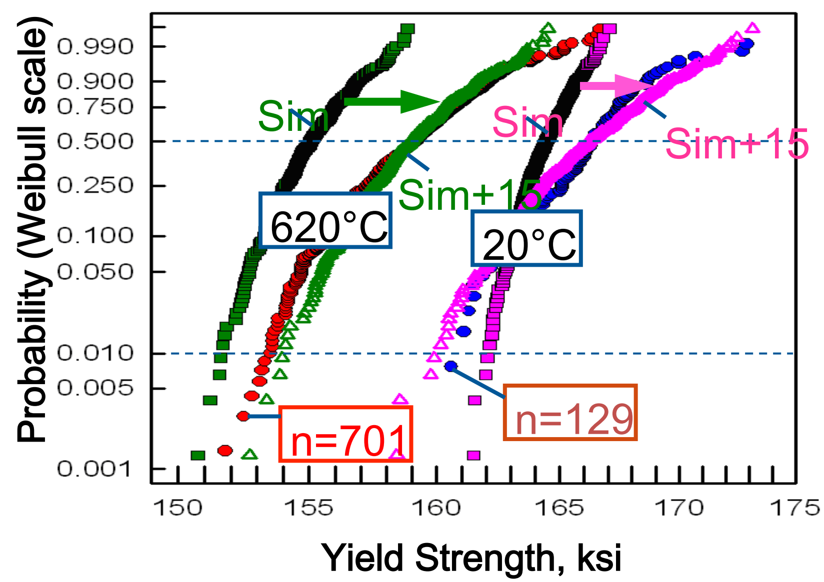
Integration, Accelerated Insertion of Materials

DARPA AIM Accelerated Insertion of Materials

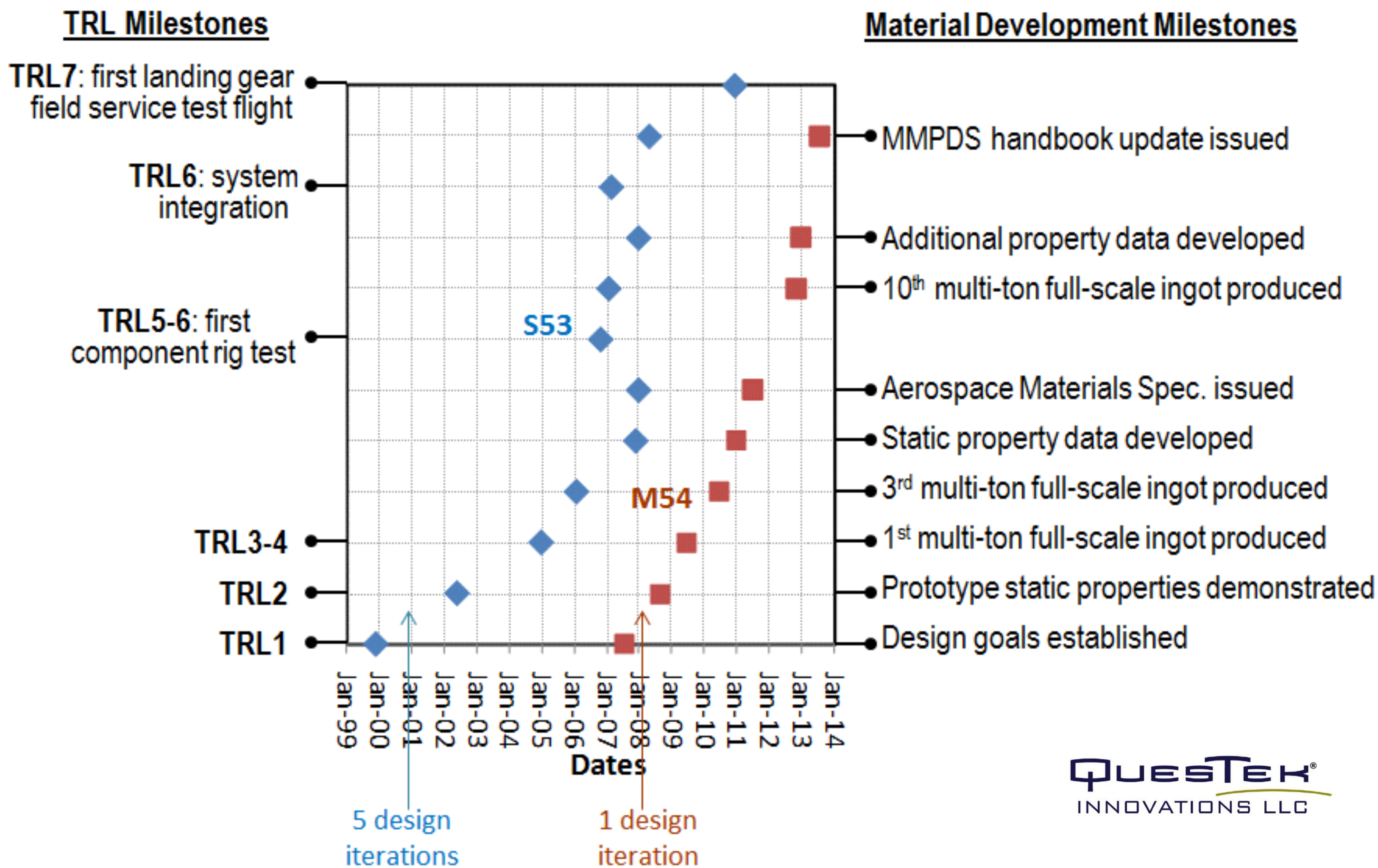








Computational Materials Qualification Acceleration



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