DEVCOM ARL
HTMDEC

MACHINE LEARNING ENHANCED MODELS FOR MATERIALS @ EXTREME CONDITIONS: HYPERSONICS & PROTECTION

Ale Strachan,* Ilias Bilionis, Marisol Koslowski, Michael Titus, Greg Wagner

Purdue University & Northwestern University

* strachan@purdue.edu

Exotic phenomena at extreme conditions

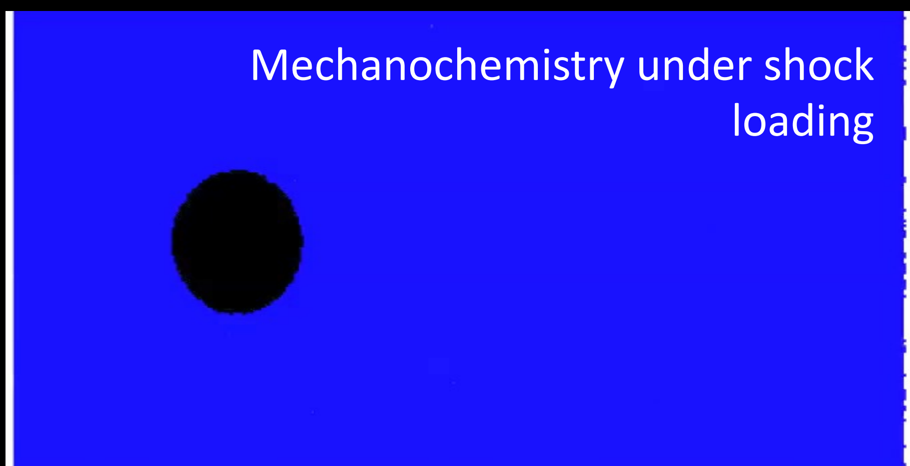
PNAS

Virtual melting as a new mechanism of stress relaxation under high strain rate loading

Valery I. Levitas[a,1] and Ramon Ravelo[b,c]

[a]Departments of Aerospace Engineering, Mechanical Engineering, and Material Science and Engineering, Iowa State University, Ames, IA 50011; [b]Physics Department and Materials Research Institute, University of Texas, El Paso, TX 79968; and [c]Computational Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545

13204–13207 | PNAS | August 14, 2012 | vol. 109 | no. 33



Polymers misbehaving

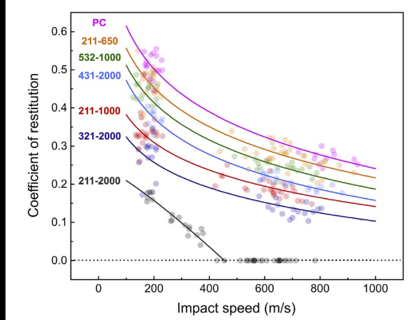


Fig. 6. Coefficient of restitution as a function of impact speed for select model PUU elastomers and PC.

Rubbers behaving like glasses

Veysset et al. Polymer (2017)

Journal of Applied Physics

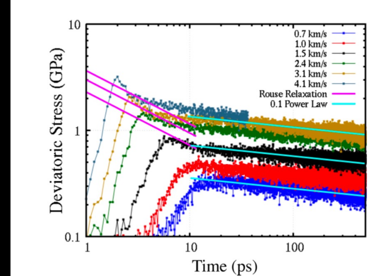
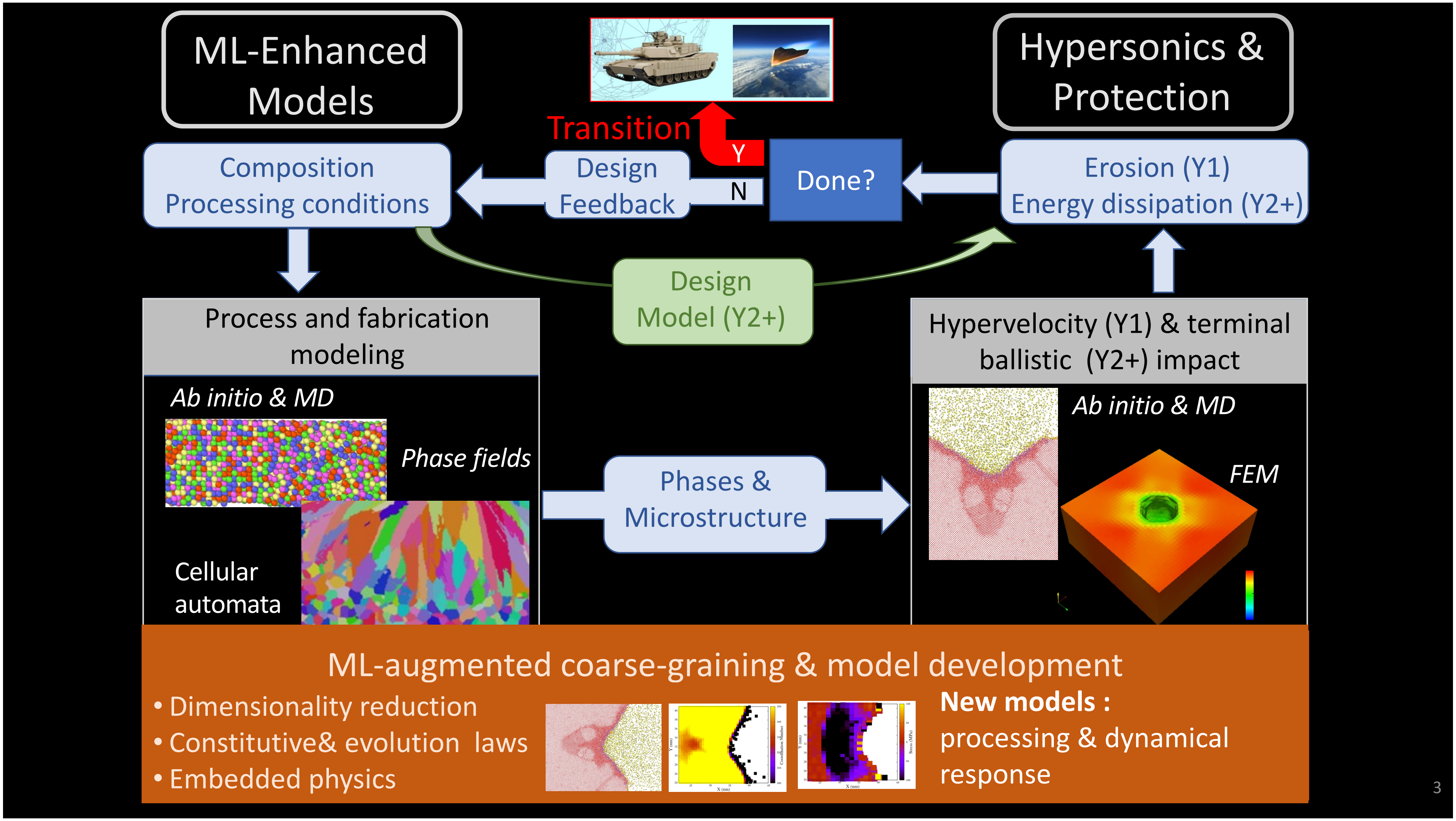
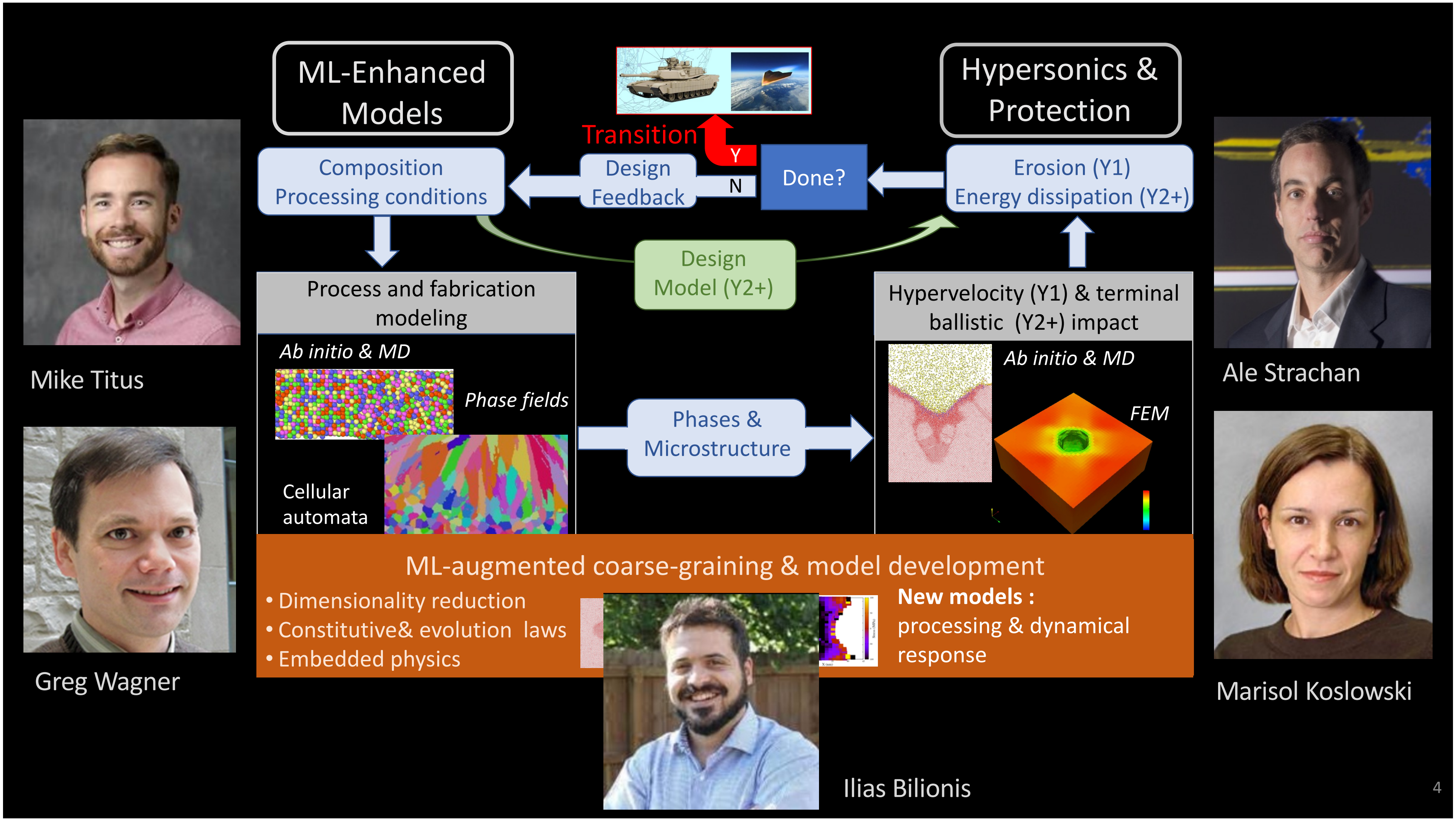


FIG. 1. von Mises stress time histories for several u_p shocks. Magenta lines represent the expected decay rates of a Rouse mode relaxation in an unentangled melt for various pre-factors. The cyan lines are similar power law decays with an exponent of −0.1.

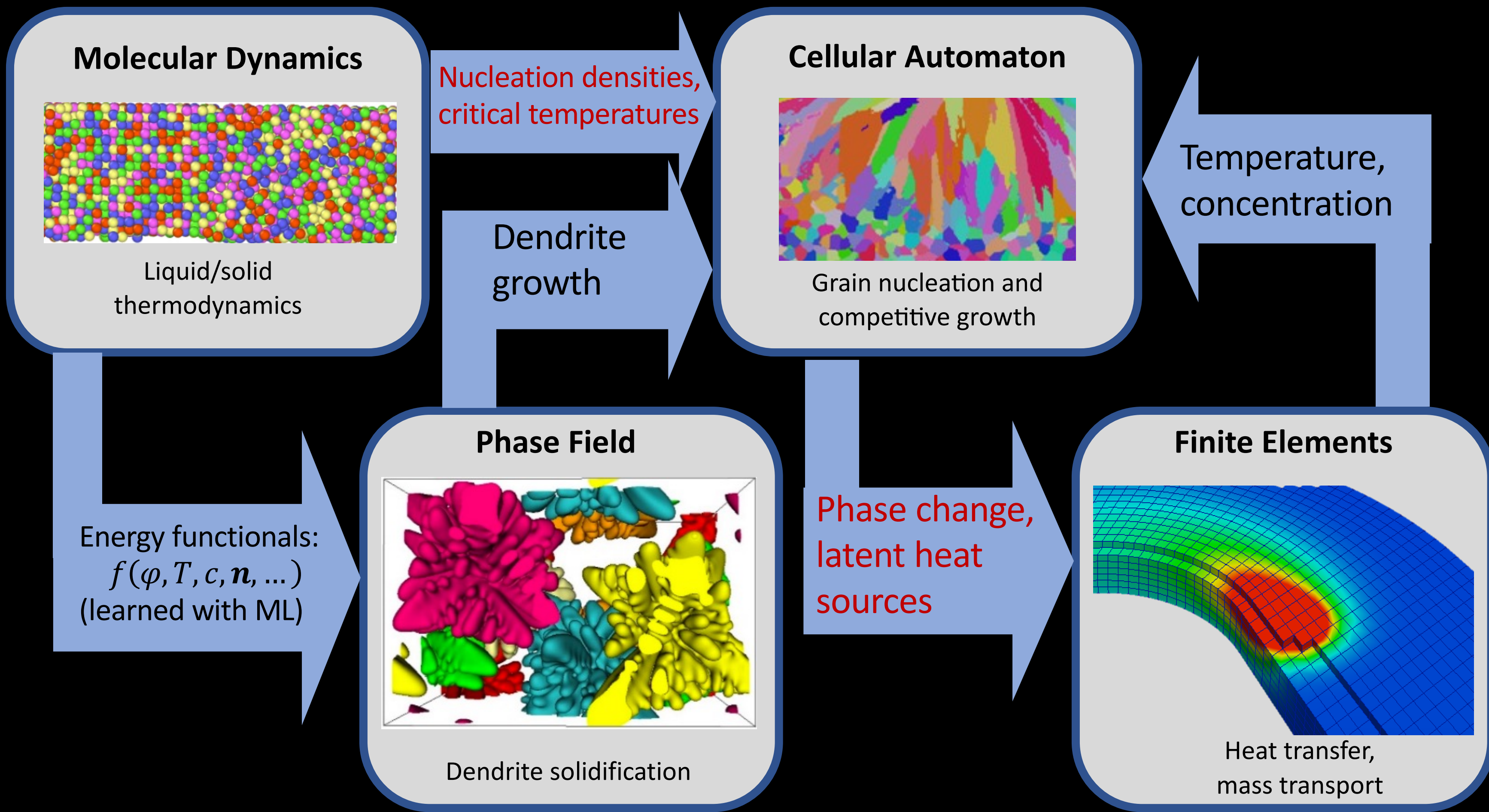
Shock-induced transient melting in glasses

Macatangay, Hamilton, Strachan (in press)


ML-Enhanced Models
Hypersonics & Protection
Transition
Y
N
Composition
Processing conditions
Design Feedback
Done?
Erosion (Y1)
Energy dissipation (Y2+)
Design Model (Y2+)
Process and fabrication modeling
Ab initio & MD
Phase fields
Cellular automata
Phases & Microstructure
Hypervelocity (Y1) & terminal ballistic (Y2+) impact
Ab initio & MD
FEM
ML-augmented coarse-graining & model development
• Dimensionality reduction
• Constitutive& evolution laws
• Embedded physics
New models :
processing & dynamical response

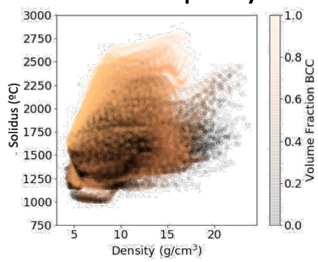

ML-Enhanced Models
Hypersonics & Protection
Transition
Y
N
Composition Processing conditions
Design Feedback
Done?
Erosion (Y1) Energy dissipation (Y2+)
Design Model (Y2+)
Process and fabrication modeling
Ab initio & MD
Phase fields
Cellular automata
Phases & Microstructure
Hypervelocity (Y1) & terminal ballistic (Y2+) impact
Ab initio & MD
FEM
ML-augmented coarse-graining & model development
• Dimensionality reduction
• Constitutive& evolution laws
• Embedded physics
New models :
processing & dynamical response
Mike Titus
Greg Wagner
Ale Strachan
Marisol Koslowski
Ilias Bilionis
4

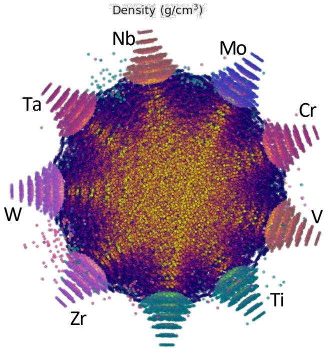
Thrust 1: process and fabrication modeling



Y1 deliverables: processing models for BCC alloys

High-throughput
CALPHAD + Property Models

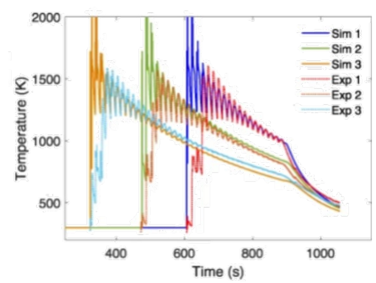


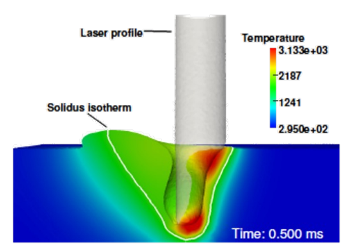


$c_i, T \rightarrow \rho, c_p, \kappa, \Delta H_f, T_s, T_L, \epsilon$

Surrogate models
for inverse design

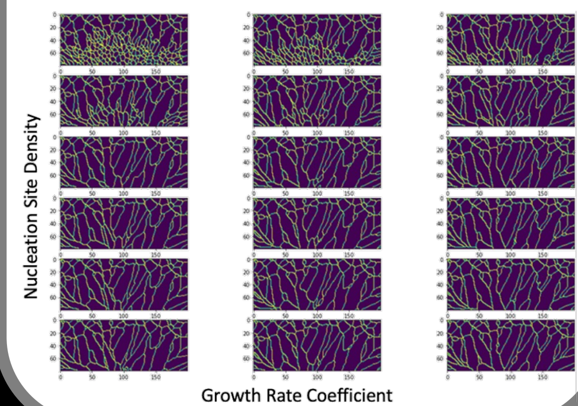
Thermal Models





$f(x, t | T_0, P) \rightarrow G, V_T, R$

Microstructure Models
via Cellular Automaton

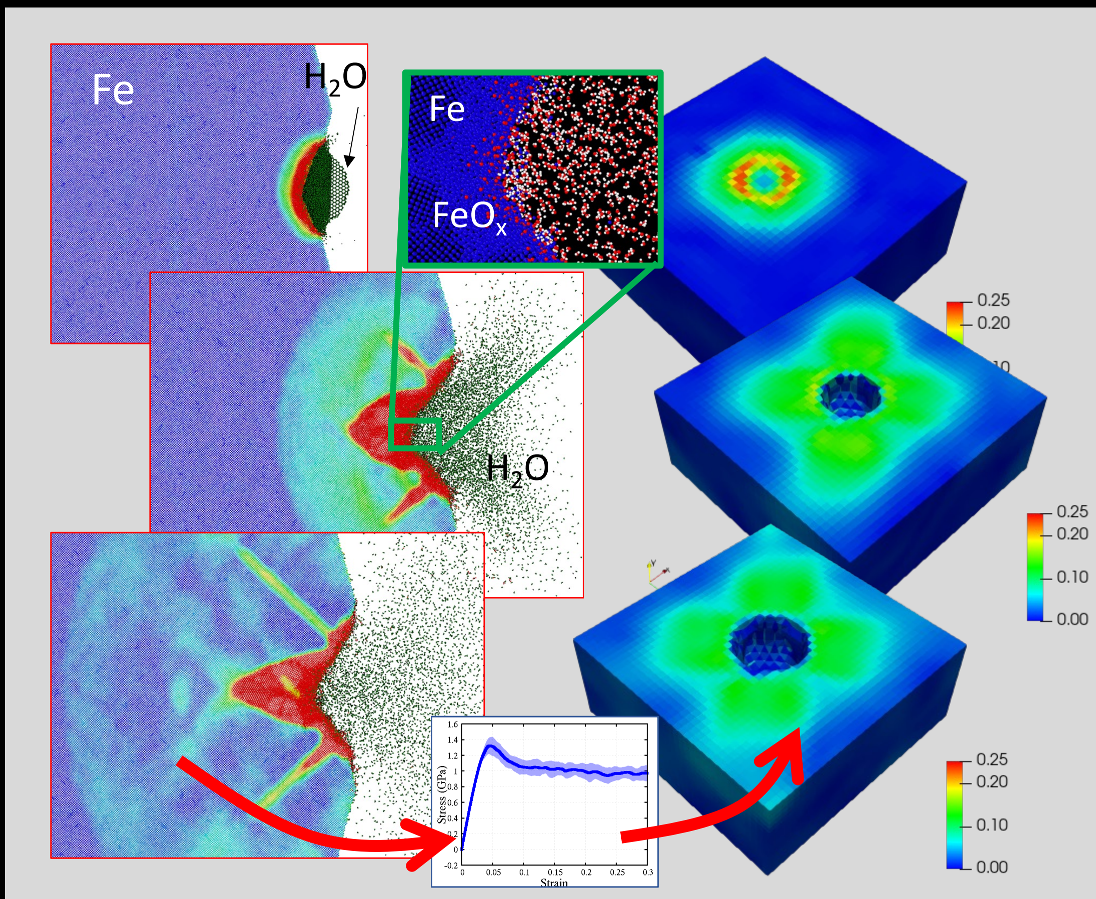


Texture, Grain Size, Anisotropy

<u>Materials of Interest</u>

- Y1: BCC-based alloys
- Y2+ MMCs fabricated via solidification

Thrust 2: Hypervelocity & ballistic impact



- Shocks & EOS
- Plasticity (rate & pressure effects)
- Phase transformations (solid-solid & melting
- Fragmentation & jetting
- Chemistry

Need for improved models

Contents lists available at ScienceDirect

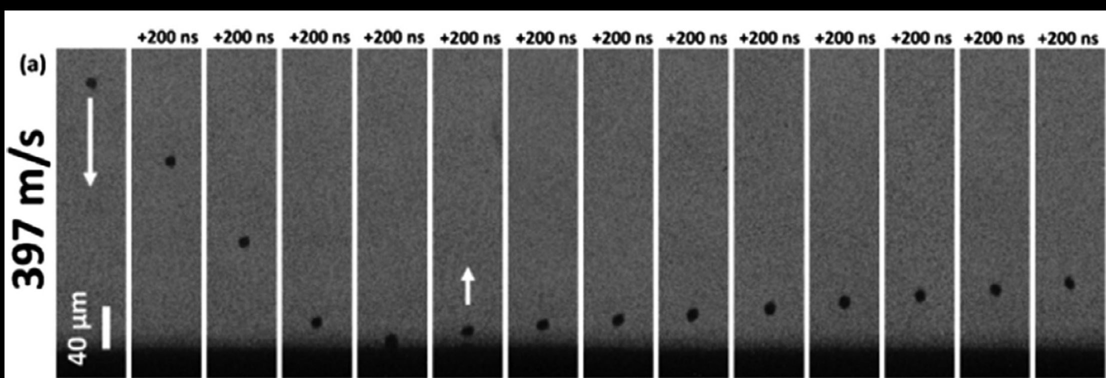
Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

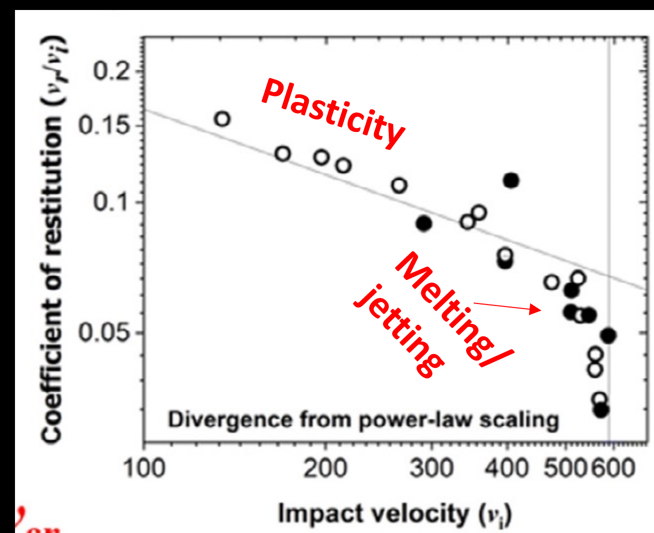
Site-specific study of jetting, bonding, and local deformation during high-velocity metallic microparticle impact

Ahmed A. Tiamiyu[a], Yuchen Sun[a,b,c], Keith A. Nelson[b,c], Christopher A. Schuh[a,1,*]

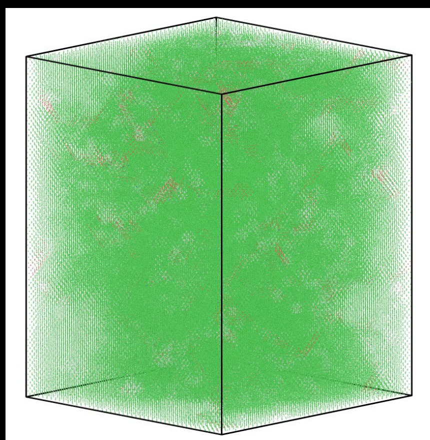
[a] Department of Materials Science and Engineering, MIT, Cambridge, MA, 02139, USA
[b] Institute for Soldier Nanotechnologies, MIT, Cambridge, MA, 02139, USA
[c] Department of Chemistry, MIT, Cambridge, MA, 02139, USA



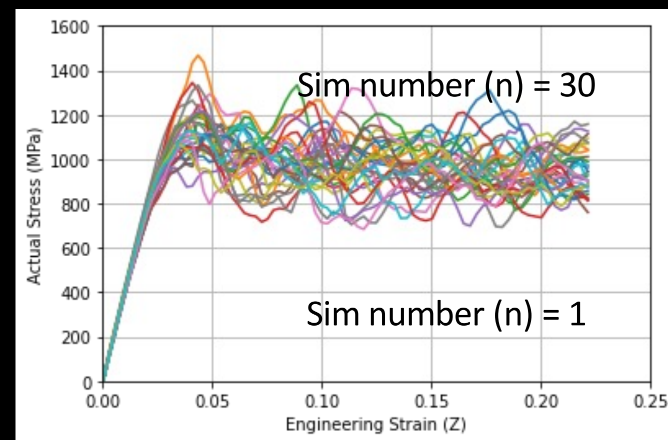
Existing plasticity models cannot capture the plastic region

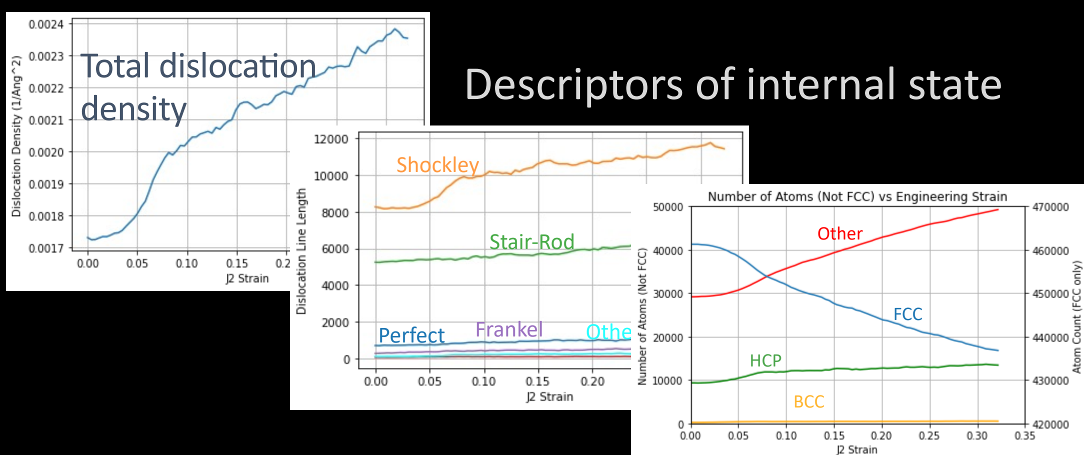


Y1 deliverables: high-strain rate models for metals



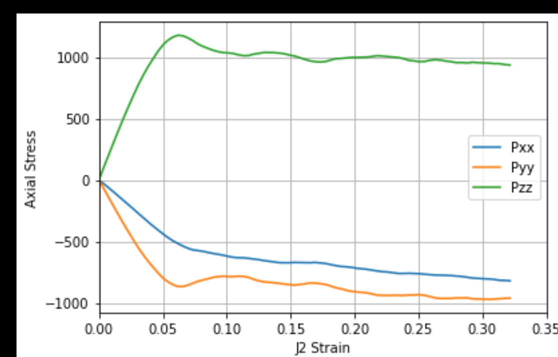
- 10 triaxial deformation paths
- Characterize fluctuations
- Strain rates 10^8-10^7 1/s
- Initial dislocation structure
- Single-element alloys and BCC HEAs





Descriptors of internal state

Stress



Thrust 3: ML-enhanced coarse-graining

Fine-scale simulations

⬇

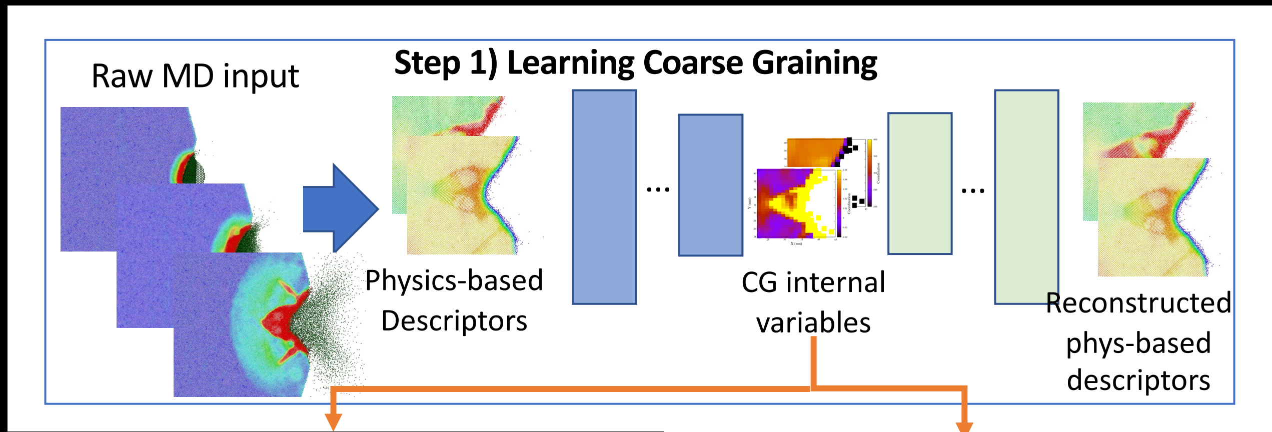
Retain CG variables based on intuition & physics

⬇

Models for the evolution of the CG variables

⬇

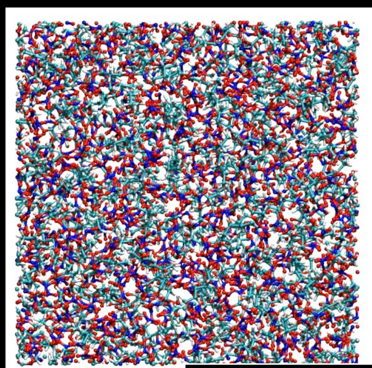
Model parameterization



Example of ML-enhanced coarse graining

Coarse graining

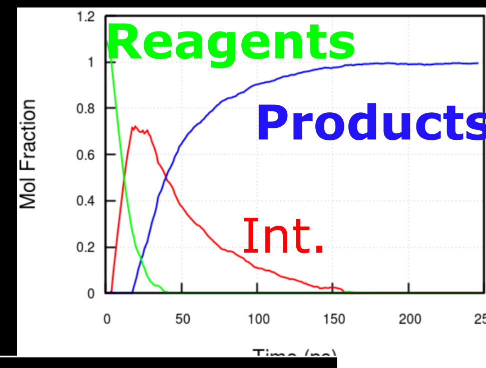
Detailed chemistry



Dimensionality reduction

Non-negative matrix factorization

Reduced chemistry



Machine learning approach for dimensionality reduction CAN lead to interpretable models

RDX —

(mole fractions)

$$\dot{Y}_1 = -Y_1 Z_a \exp(-\frac{E_a}{RT})$$

$$\dot{Y}_2 = Y_1 Z_a \exp\left(-\frac{E_a}{RT}\right) - Y_2 Z_b \exp(-\frac{E_b}{RT})$$

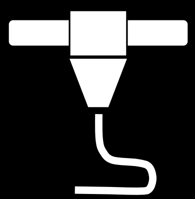
$$\dot{Y}_3 = Y_2 Z_b \exp(-\frac{E_b}{RT})$$

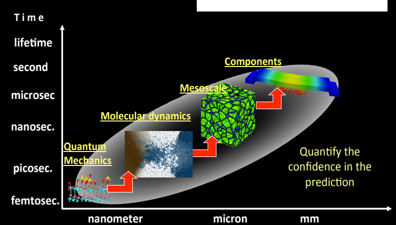
Heat evolved

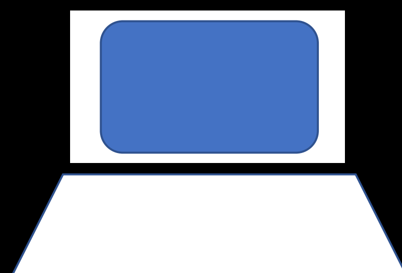
$$\rho C_v \dot{T} = -Q_1 \dot{C}_1 + Q_2 \dot{C}_3$$

Sakano, Hamed, Kober, Grilli, Hamilton, Islam, Koslowski, Strachan
The Journal of Physical Chemistry A. 2020 Oct 28;124(44):9141-55

We have a data problem







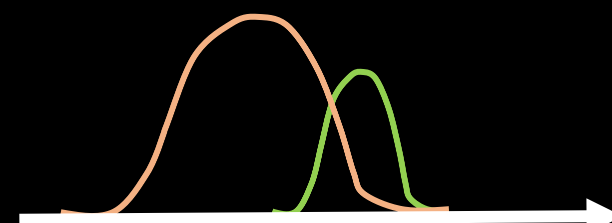
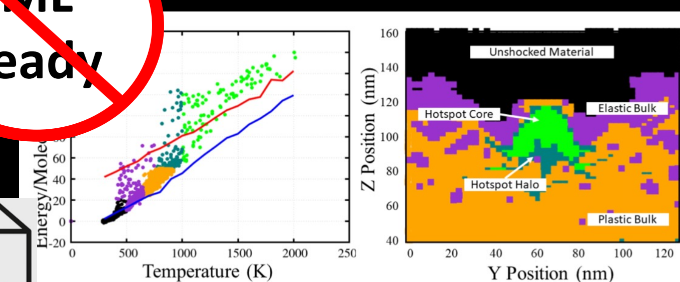
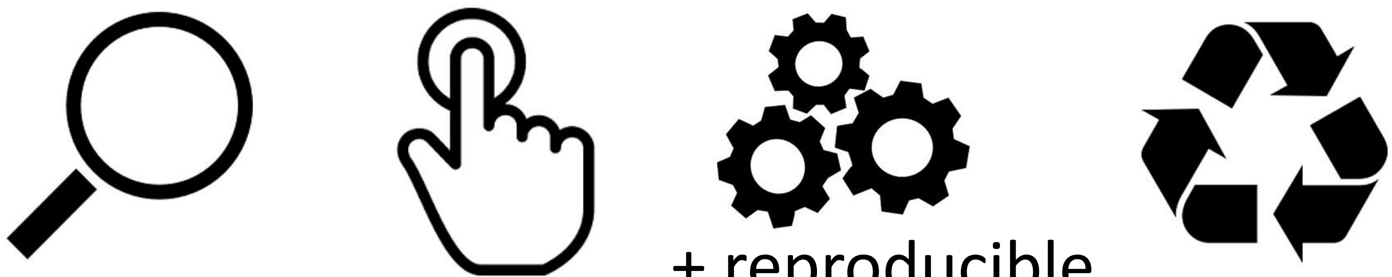


Table 1. Final Product Amounts for LLM-105 Using ReaxFF, Compared to Values for TATB and HMX[93,94]

molecule	ReaxFF-2018 (mol/cm^3)	ReaxFF-LG (mol/cm^3)	LLM-105 Cheetah (mol/cm^3)	ReaxFF-LG TATB (mol/cm^3)	TATB Cheetah (mol/cm^3)	TATB exp. (mol/cm^3)	HMX Cheetah (mol/cm^3)	HMX exp. (mol/cm^3)
N_2	1.109×10^{-2}	2.145×10^{-2}	2.604×10^{-2}	1.66×10^{-2}	2.17×10^{-2}	1.75×10^{-2}	2.47×10^{-2}	2.37×10^{-2}
CO_2	1.313×10^{-2}	5.280×10^{-3}	1.297×10^{-2}	2.80×10^{-3}	1.20×10^{-2}	1.46×10^{-2}	1.24×10^{-2}	1.24×10^{-2}
H_2O	3.335×10^{-4}	7.442×10^{-3}	1.440×10^{-2}	1.05×10^{-2}	1.89×10^{-2}	1.56×10^{-2}	1.88×10^{-2}	2.05
NH_3	2.264×10^{-3}	1.783×10^{-3}	1.194×10^{-3}	3.07×10^{-3}	1.64×10^{-3}	8.23×10^{-4}	1.97×10^{-3}	2.55



Findable Accessible Interoperable Reusable



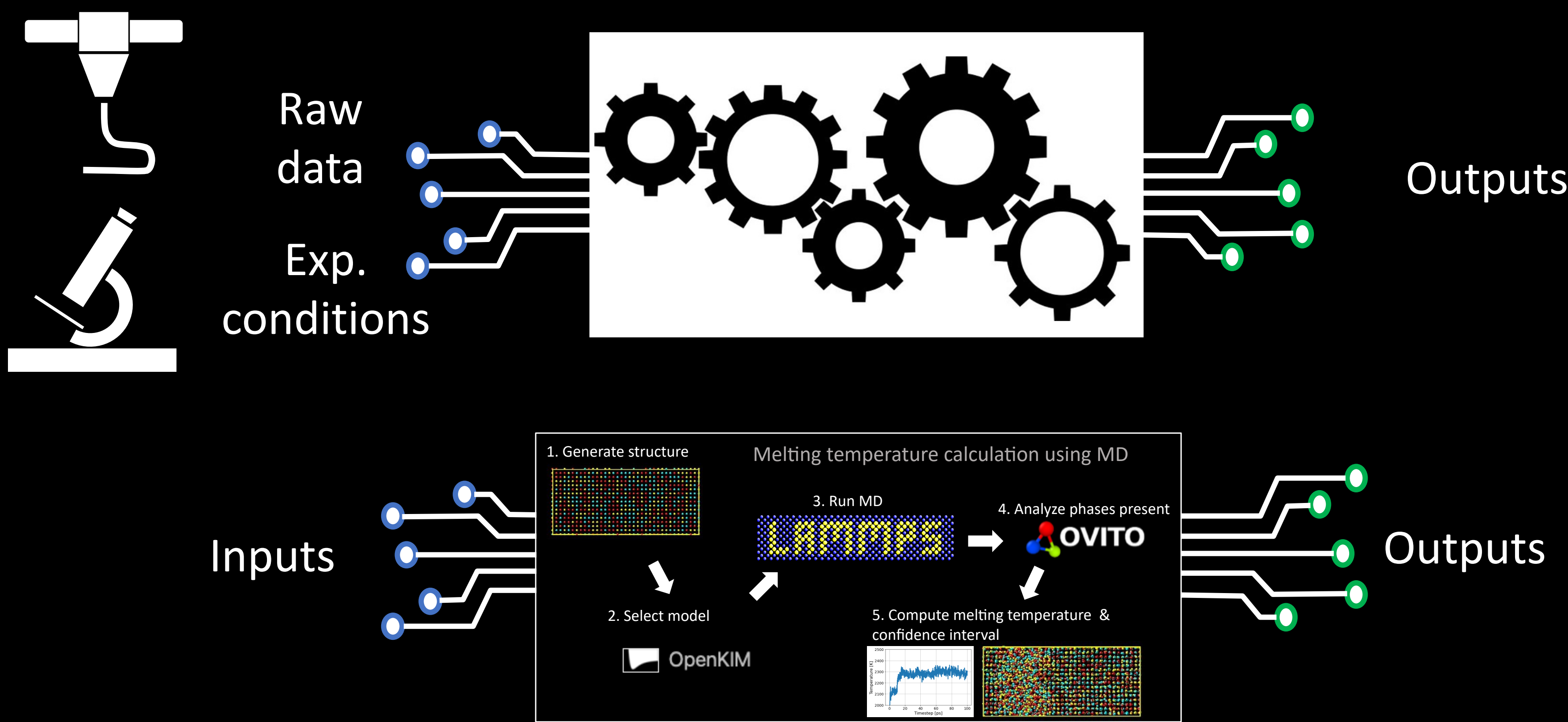
+ reproducible

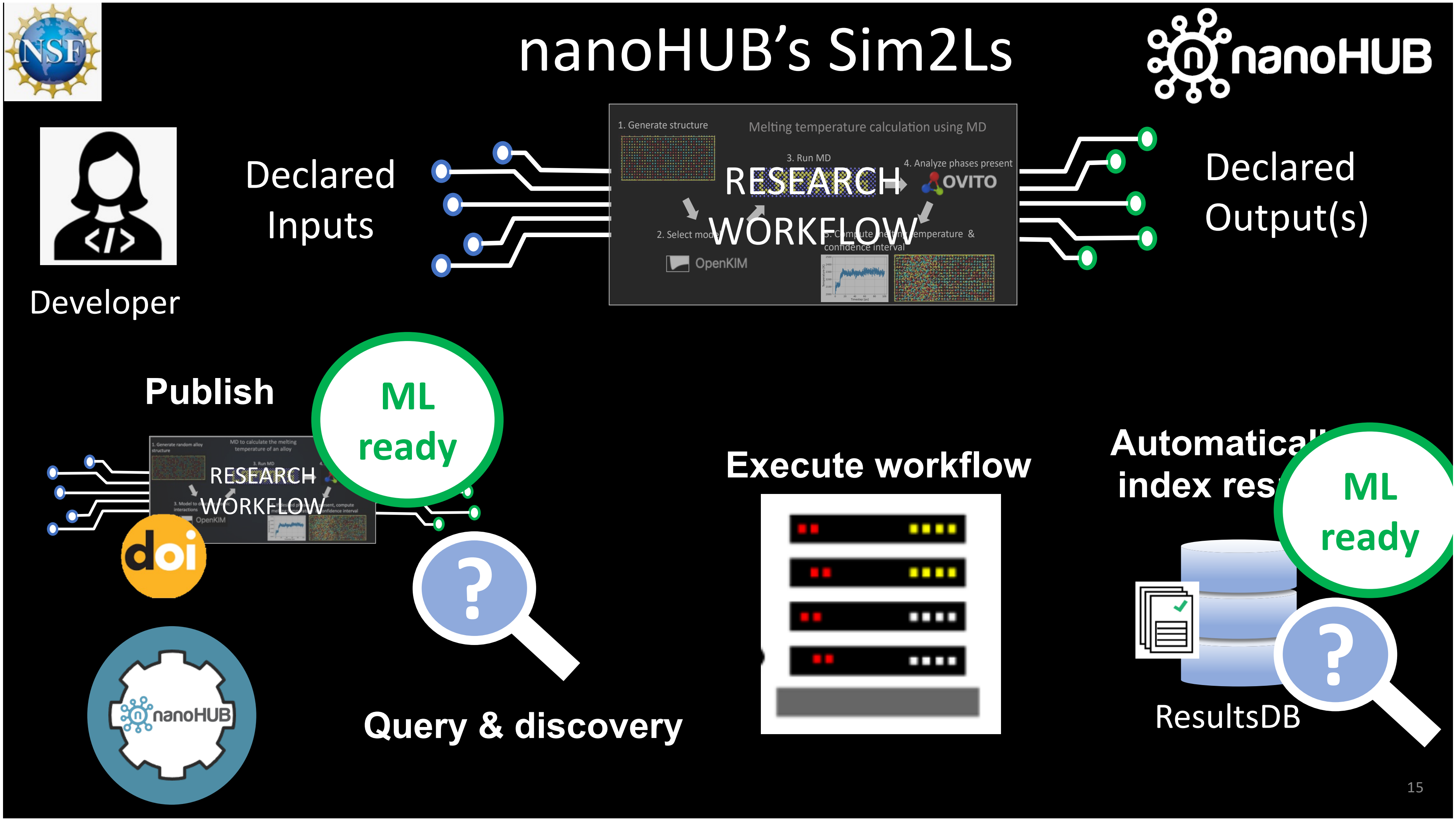
MaRDA

ML, analysis, & simulation workflows

Wilkinson, et al. (2016). The FAIR Guiding Principles for scientific data management and stewardship. Scientific data, 3(1), 1-9.

Research/data workflows




nanoHUB's Sim2Ls
nanoHUB
Developer
Declared
Inputs
1. Generate structure
Melting temperature calculation using MD
3. Run MD
4. Analyze phases present
RESEARCH
WORKFLOW
OVITO
2. Select model
OpenKIM
Declared
Output(s)
Publish
ML
ready
RESEARCH
WORKFLOW
doi
nanoHUB
Query & discovery
Execute workflow
Automatically
index res
ML
ready
ResultsDB
15

Collaborations with DEVCOM ARL & HTMDEC seedlings

- Advanced manufacturing of metallic alloys & cermets
  - Processing – microstructure relationships

- Hyper-velocity impact and erosion experiments

- Data science and materials informatics
  - FAIR data & workflows

- Multiscale modeling of materials at extreme conditions
  - Rate and high-pressure effects on plasticity & fracture
  - Chemistry