Multiscale Simulation Framework for Modeling of Structural Energetics

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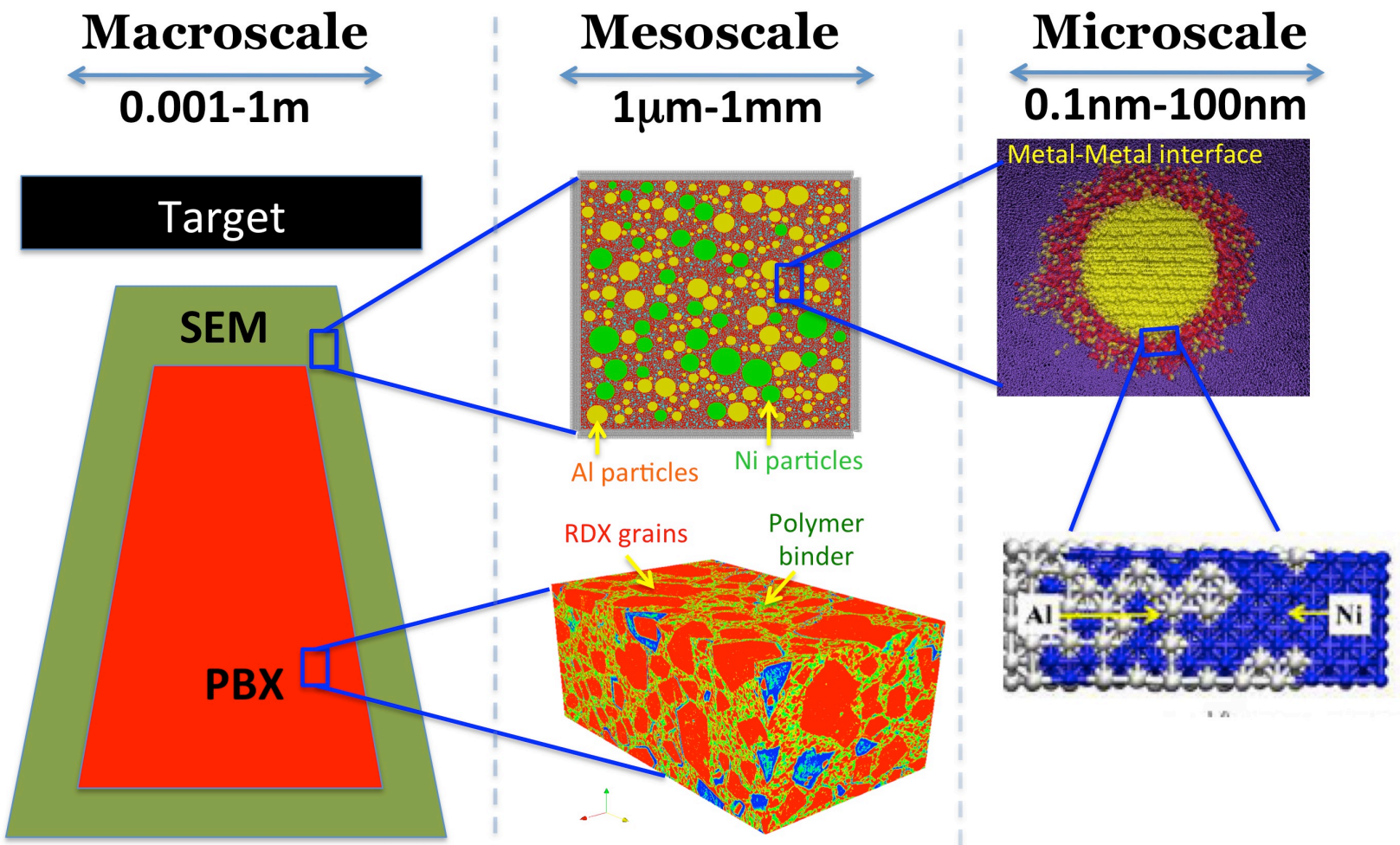
Objectives of Phase-I

1) **Capitalize on our extensive experience in multiscale modeling simulations of energetic materials using and adopt/enhance this approach for investigation and design of structural energetic materials (SEMs).**

2) **Using this multiscale modeling approach to identify and study key phenomena (and their coupling) that define the response of SEM under various insult scenarios.**

Multiscale modeling approach



MPM-ICE

Homogenized and stochastically heterogeneous burn models and mechanical properties of SEM, PBX, product gases and target.

MPM, MPM-ICE

Heterogeneous structure of SEM, PBX is resolved + heterogeneous burn models.

Reactive and classical MD simulations

Data to parameterize friction, burn, damage, and mechanical models.

Materials Point Method + Uintah Computational Framework

(12+ years development under DOE ASCI program C-SAFE at UofU)

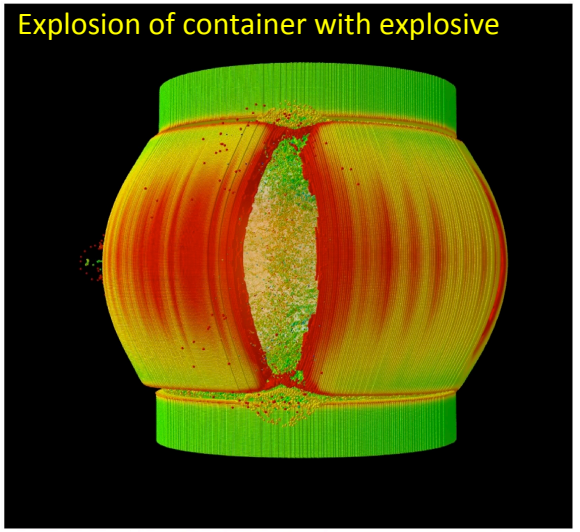
-MPM is a mixed grid /particle method

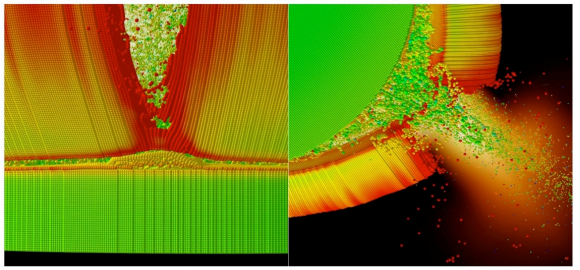
-Excellent for large deformations, multi-phase and multi-material systems

-Includes coupling of fluid-solid interactions (MPM-ICE)

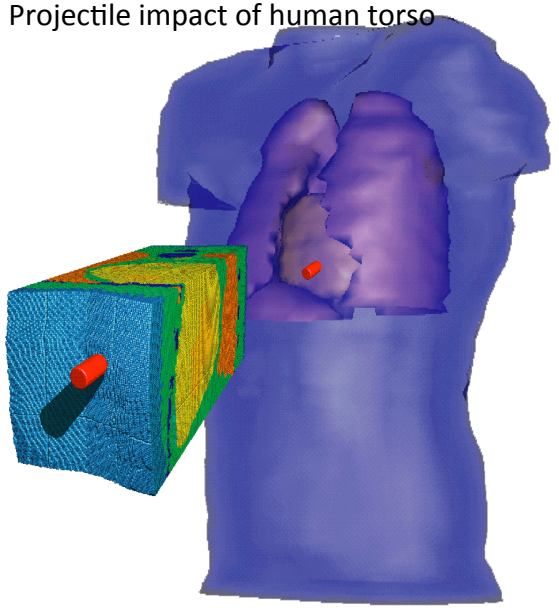
-Adaptive mesh refinement

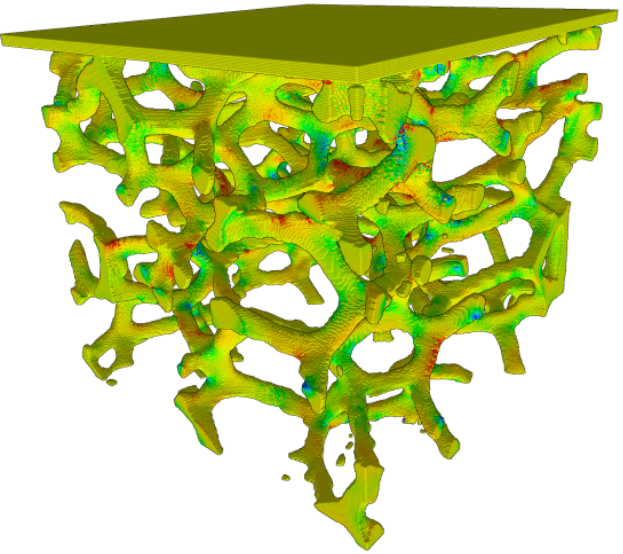
-MPM+Uintah are highly scalable (up to 1M cores)



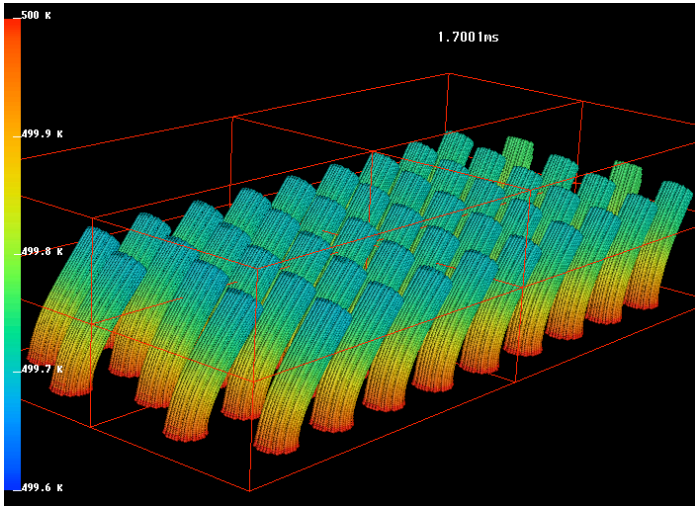


Projectile impact of human torso





Compaction of a foam

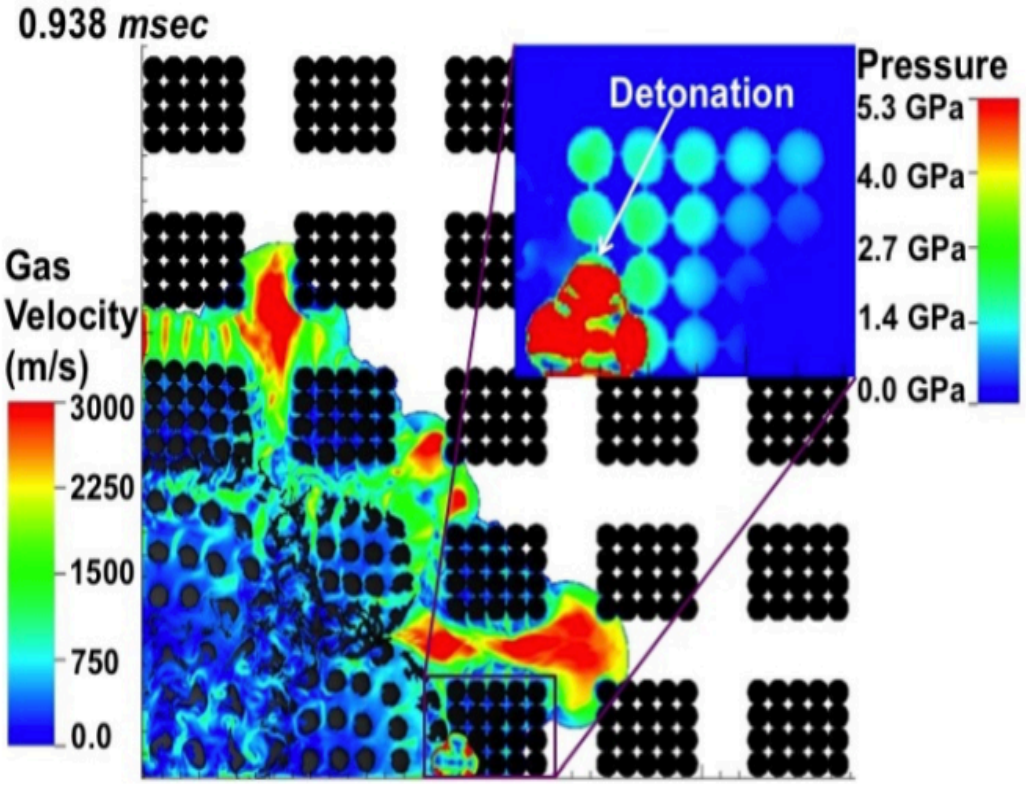


Fluid-structure interaction in microfluidic device

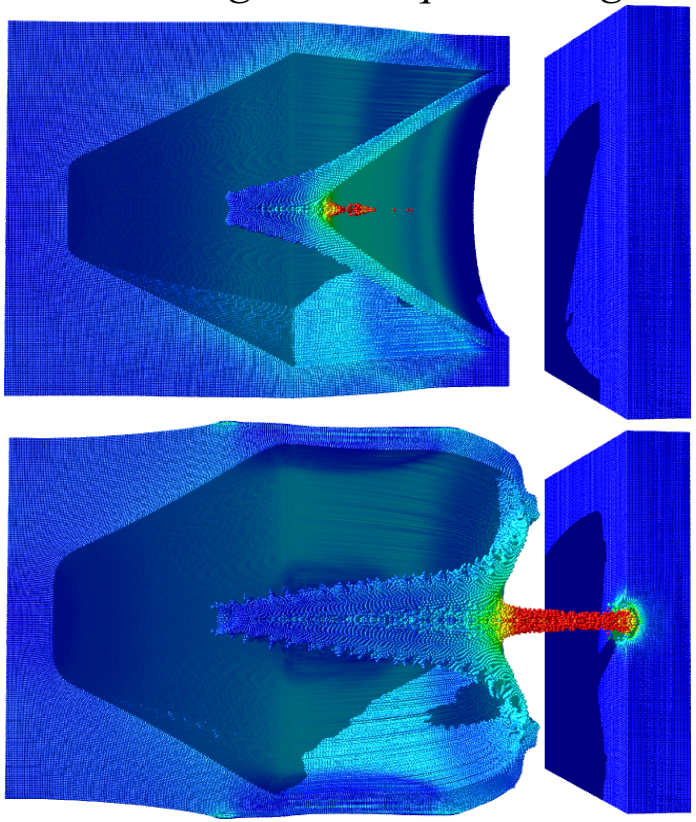
Materials Point Method + Uintah

(recent applications/developments)

Solid/gas interactions in an exploding array of homogenized PBX-9501 cylinders



MPM simulation of shape-charge driven penetration of tungsten particles into a granular quarts target.



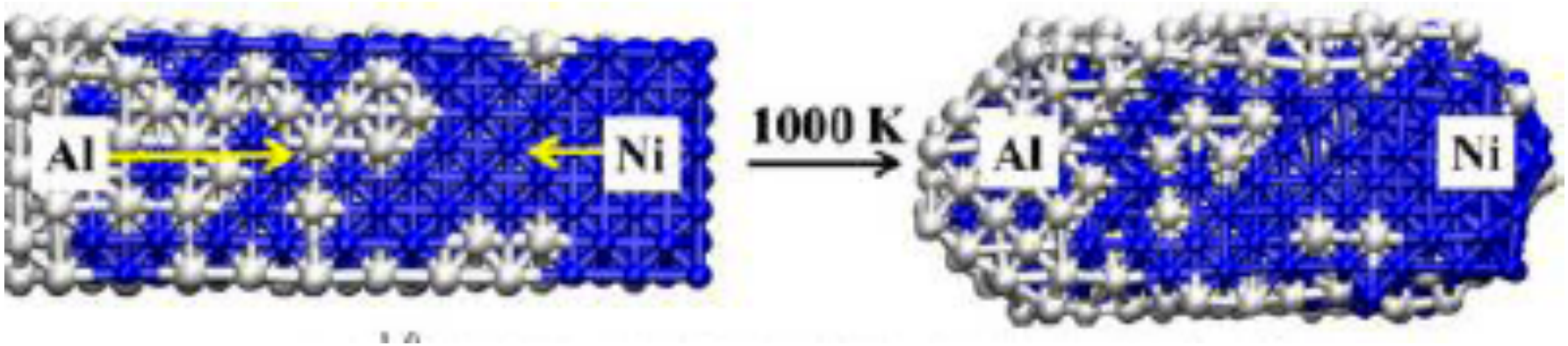
Initial formation of the tungsten particle jet via explosive initiation (top) and high velocity impact of the tungsten particles due to cohesive acceleration via the shaped shockwave interaction (bottom). Coloration indicates velocity from low (blue) to high (red).

Atomistic MD simulations

-Atoms, molecules and reactions/interactions between them are resolved explicitly

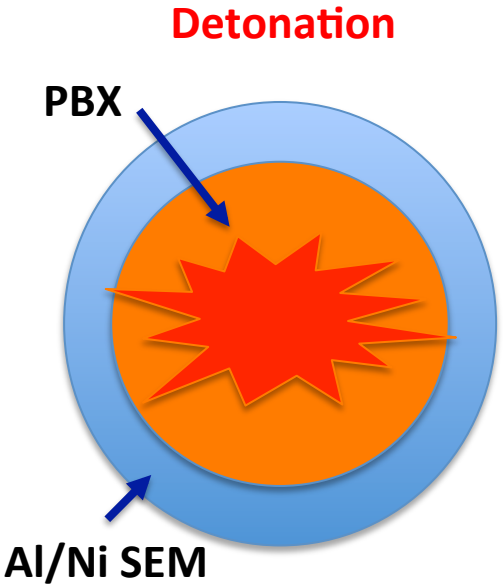
-Allow to obtain correlations between molecular scale structure and macroscopic properties

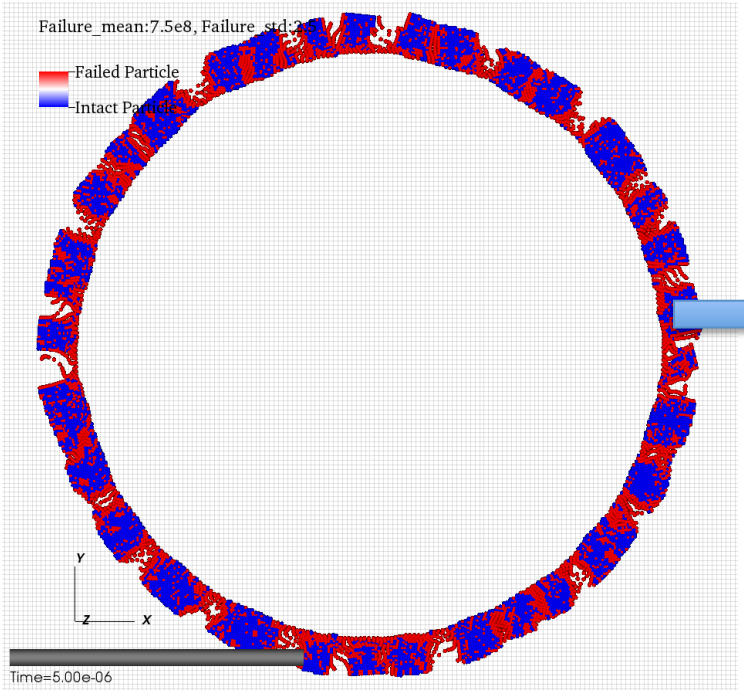
-Provide crucial insight/properties for materials/conditions hardly accessible for experiments (e.g., mechanical and reaction properties of energetic materials, interfacial properties, etc).

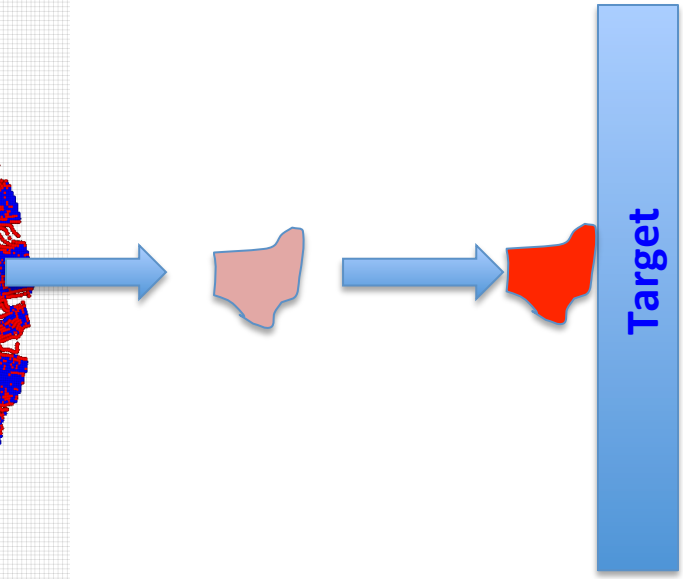


Phase I Objective: Develop and demonstrate multiscale modeling capabilities for the test case scenario:

- PBX ignites inside Al/Ni-based SEM container
- container fragments into pieces that fly away while interacting with surrounding gas/air
- Al/Ni interdiffusion/reactions are initiated upon initial shock of SEM and continue while fragments are flying
- reacting Al/Ni SEM fragments hit the target







Phase I Technical Objectives

TO-1: Generate representative mesoscale samples with high % of TMD model SEM geometries.

TO-2: Determine frictional response of metal grain contacts under loading.

TO-3: Determine mesoscopic response to uniaxial thermal and mechanical loading of model mesoscale samples.

TO-4: Develop initial Al-Ni reaction and thermodynamic transition models.

TO-5: Implement EOS, constitutive and damage models for macroscale simulations.

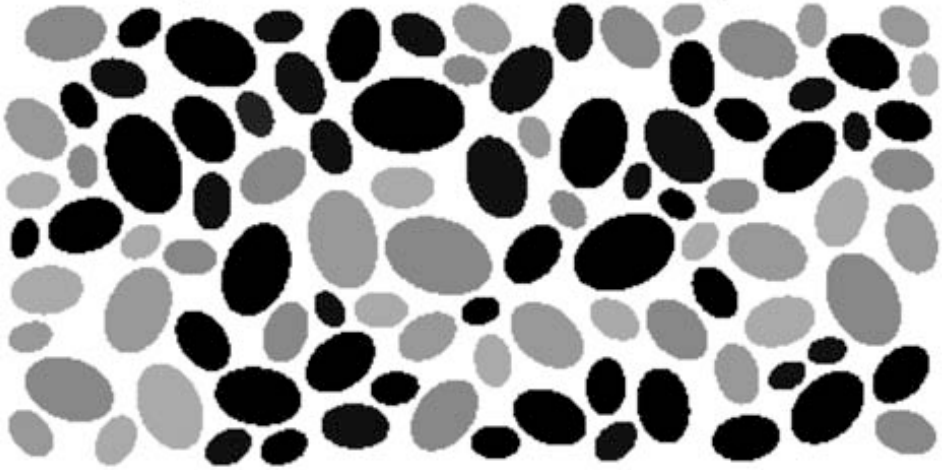
TO-6: Compare heterogeneous and homogeneous macroscale models.

Generation of Mesoscale Structures of SEM

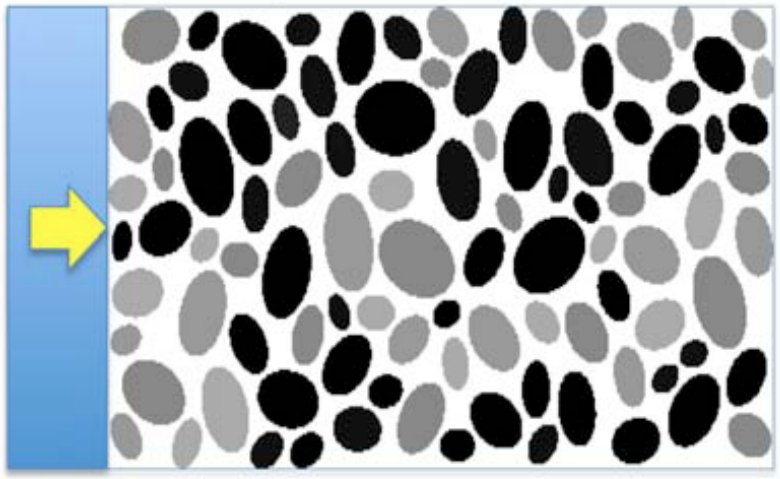
Mesoscale MPM simulations of representative SEM microstructures - -

- Fully resolved Al and Ni grains
- Realistic size distributions

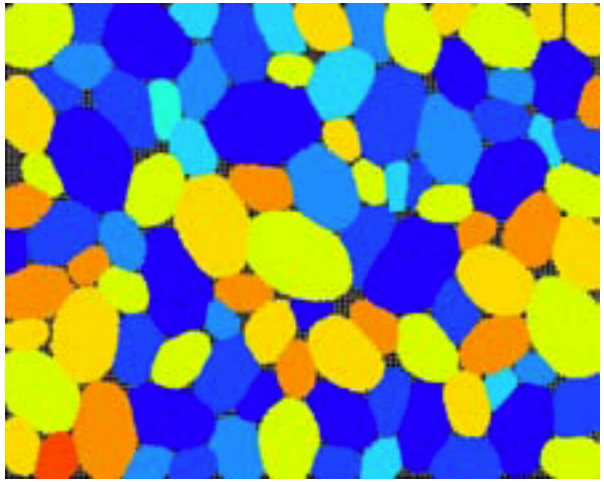
Initial configuration of Al-Ni composite, 50% TMD



Slowly compacted to desired TMD



- Final configuration from preparation ("processing") 96% TMD



Selection of models for bulk properties of SEM components

- Mie-Grueneisen EOS for Al and Ni
- Steinberg-Cochran-Guinan shear modulus for Al and Ni
- Johnson-Cook failure model for Al and Ni

Table 1. Parameters for the Mie-Grüneisen Equation-of-State for SEM Component Materials

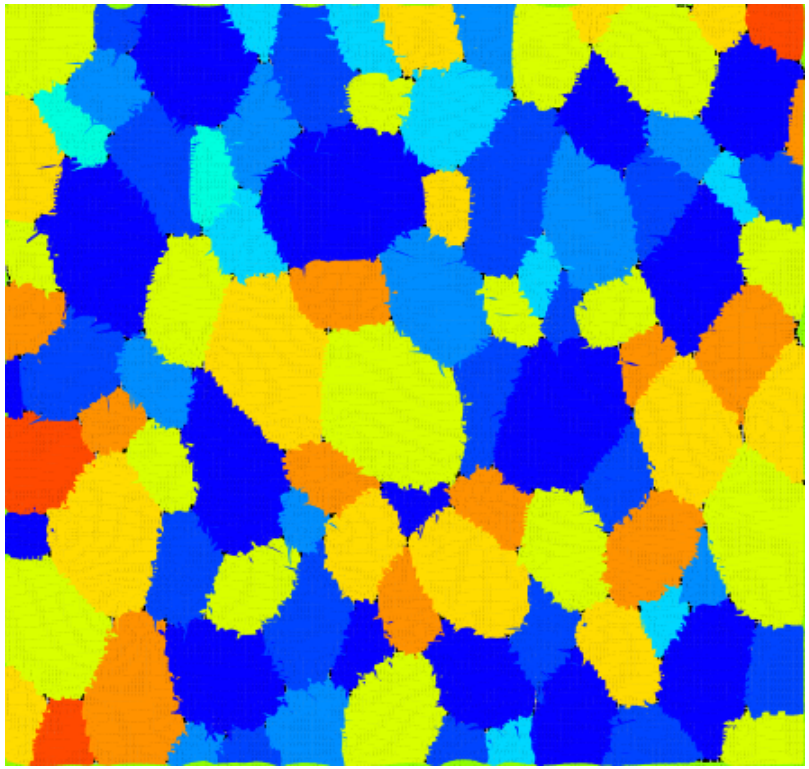
Component	ρ_R (kg/m^3)	c (m/s)	s	γ_R	K_B (Pa)	C_v (J/kgK)
Al	2780	5300	1.34	2.00	78.1E+09	920
Ni	8870	4600	1.44	1.93	188E+09	425

Table 2. Parameters for the SG Shear Modulus and JC Yield Constitutive Models for SEM Component Materials

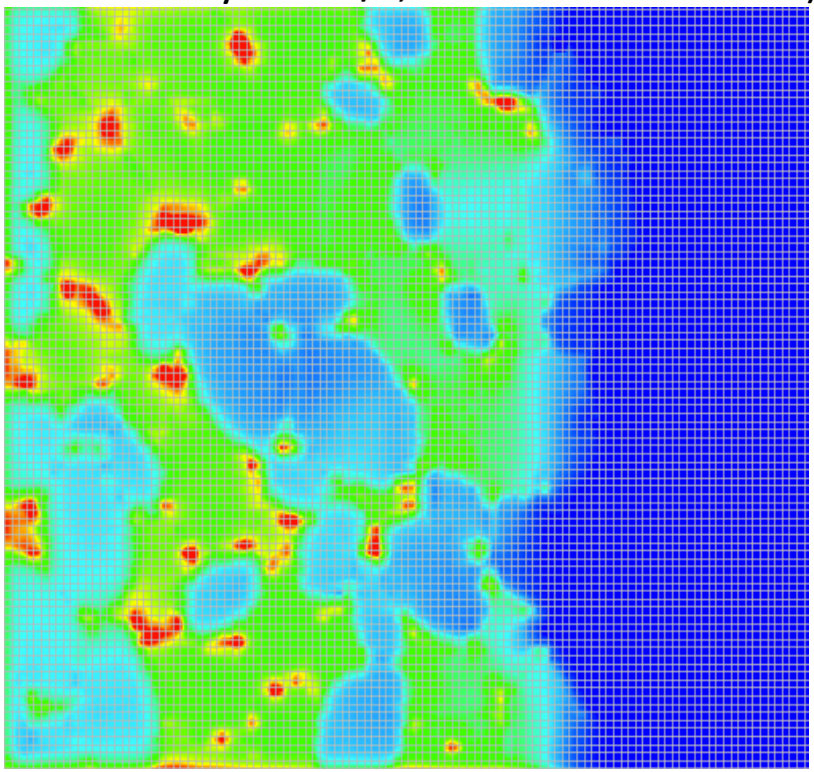
Component	G_0 *(Pa)*	G'_P/G_0 *(Pa^{-1})*	G'_T/G_0 *(K^{-1})*	A *(Pa)*	B *(Pa)*	n	C	M
Al	**27.6E+9**	**65.0E-12**	**0.62E-3**	**324.0E+6**	**114.0E+6**	**0.42**	**0.002**	**1.34**
Ni	**85.5E+9**	**16.0E-12**	**0.33E-3**	**163.4E+6**	**648.1E+6**	**0.33**	**0.006**	**1.44**

Uniaxial compression and shock of SEM

Quasistatic compression to 15GPa stress starting from a sample at 96%TMD (strain rate 40,000 1/s)



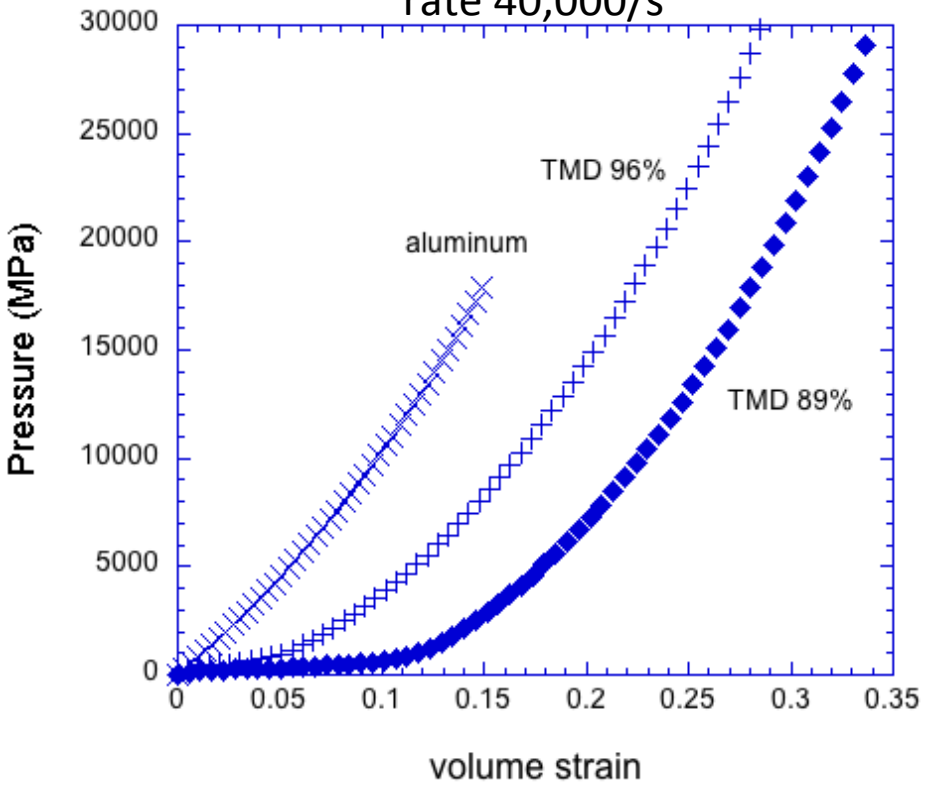
Stress distribution in the same sample after 20ns of shock propagation (shock velocity 700m/s, shock stress 15GPa)



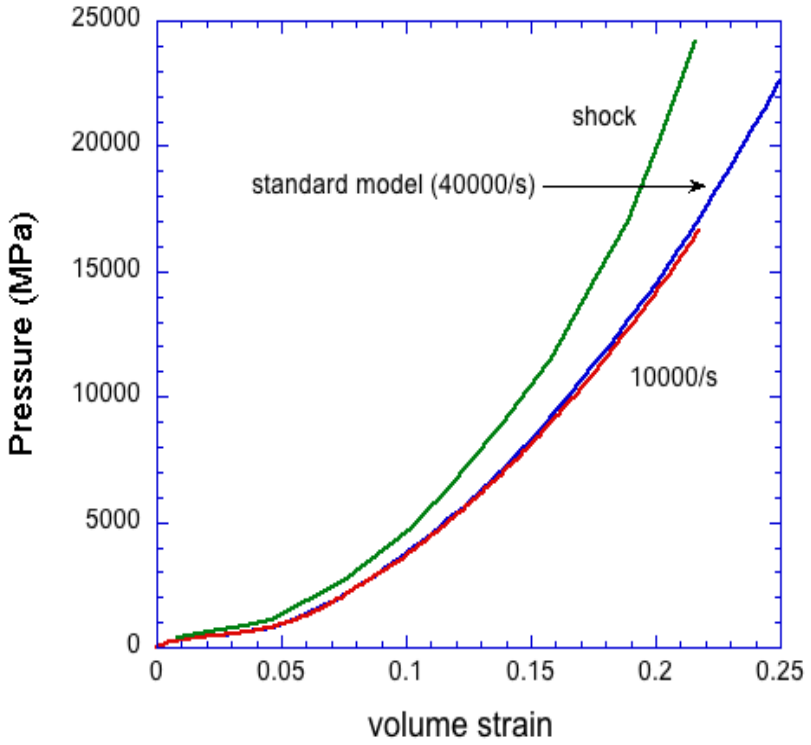
PVT behavior of SEM

- Typical behavior of granular material is observed
- Flat region is associated with “squeezing out” the void space
- The higher the strain rate the stiffer the dependence due to reduced ability of frictional sliding to allow for filling the voids

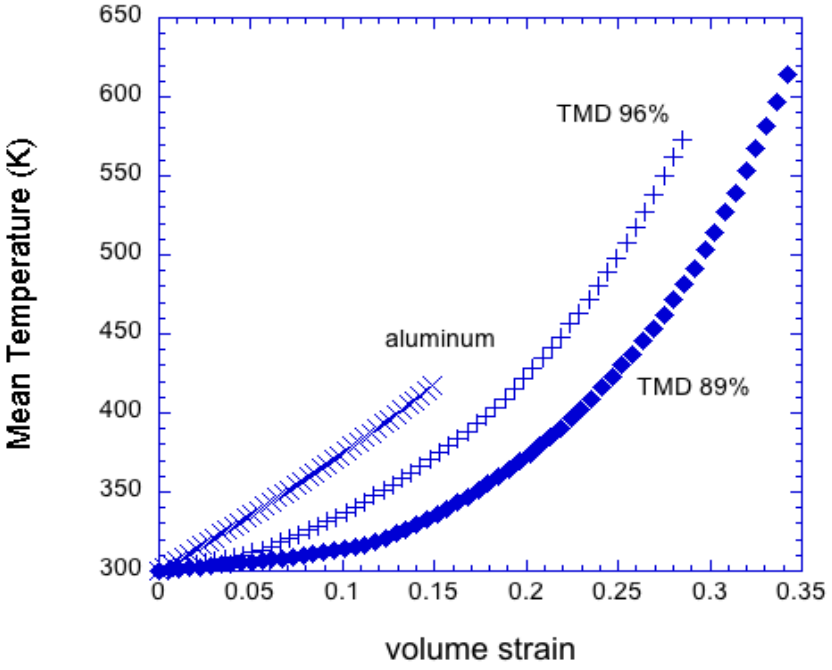
Quaistatic compression,
rate 40,000/s

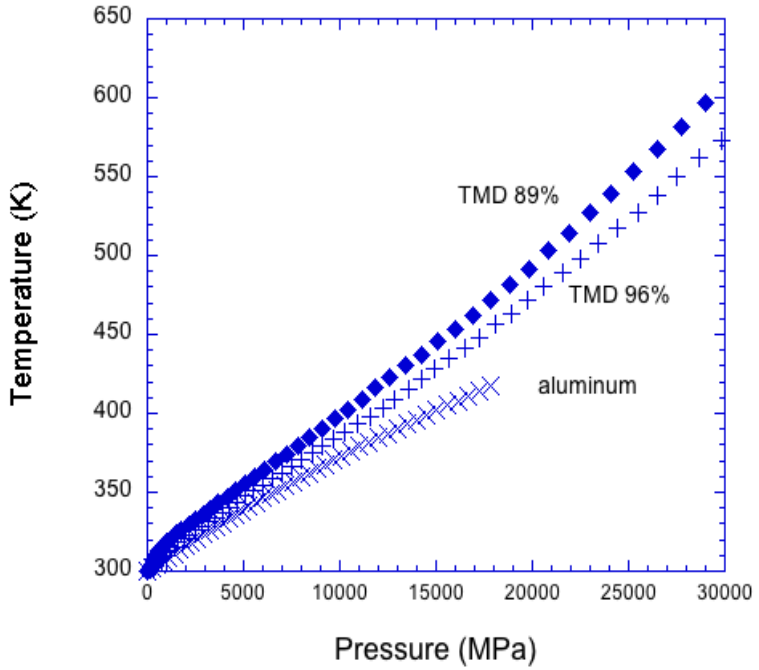


Sample with 96% TMD
Influence of strain rate



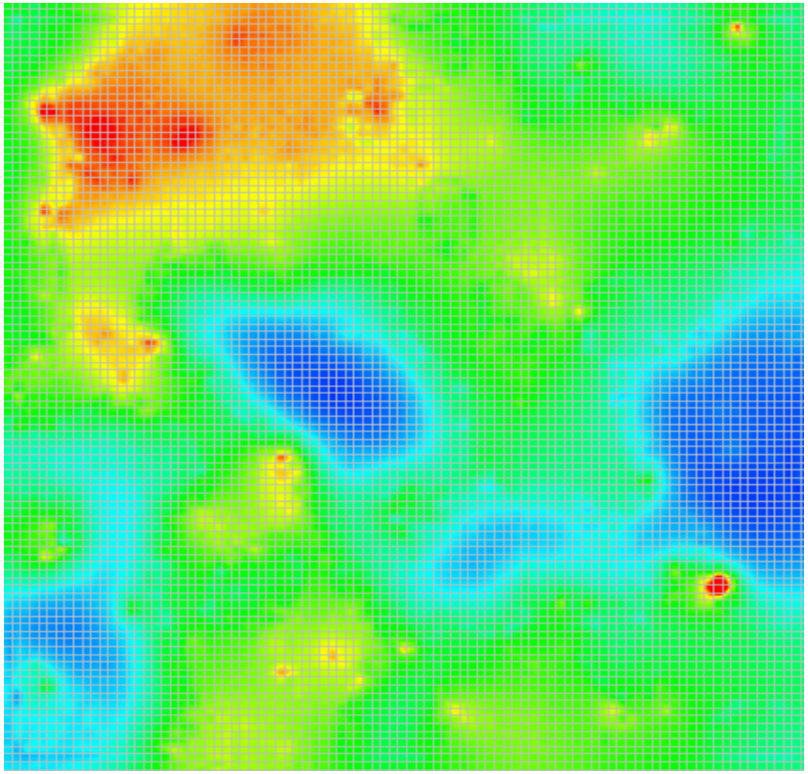
Mean temperature and temperature profiles: Quasistatic





- Friction work and plastic deformation result in modest increase of mean temperature for the range of deformations investigated.
- The mean temperature is well below the atmospheric melting temperature of aluminum (around 933 K) even for the largest deformation/highest pressures investigated.
- Note, that melting temperature of aluminum increases by about 50 K for each GPa of pressure.

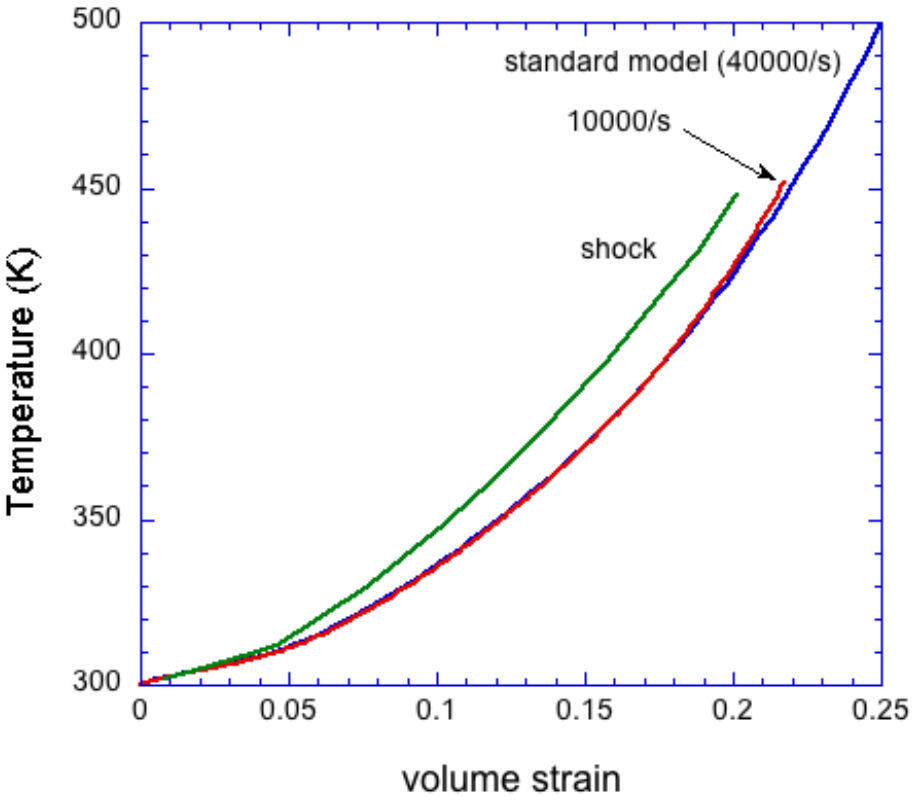
Mean temperature and temperature profiles: Quasistatic

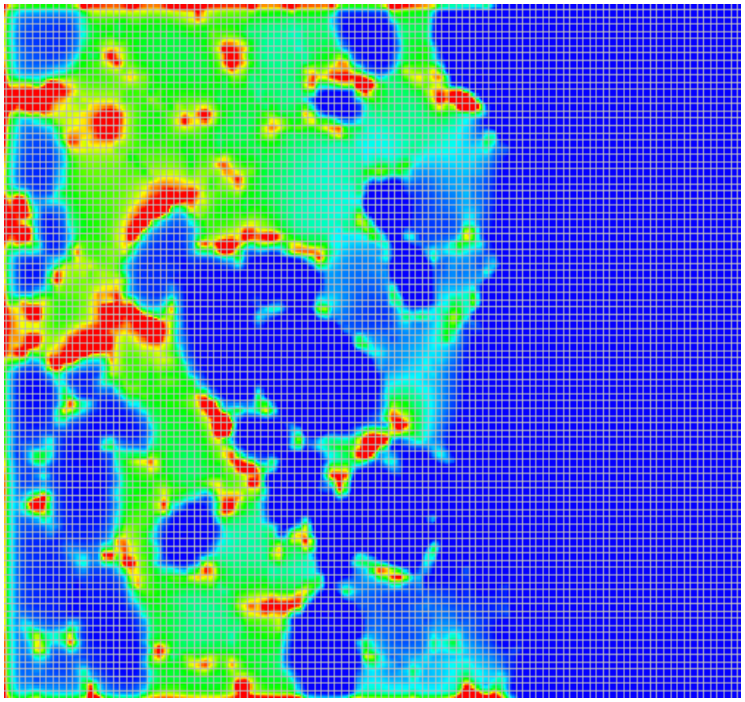


Temperature profile from the standard model after 6.2 microseconds (25 GPa) of compression. Blue to green is below mean temperature while yellow to red is above mean temperature

- Even for the significant pressure of 25 GPa, the hottest hot spots are only around 800 K, about 300 K above the mean temperature and well below aluminum melting temperature.

Mean temperature and temperature profiles: Shock

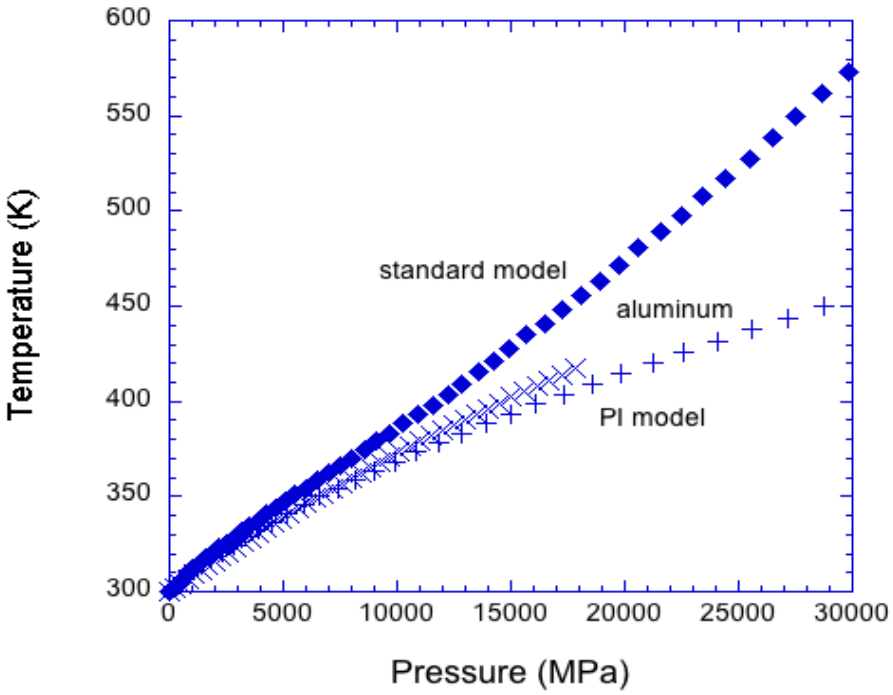


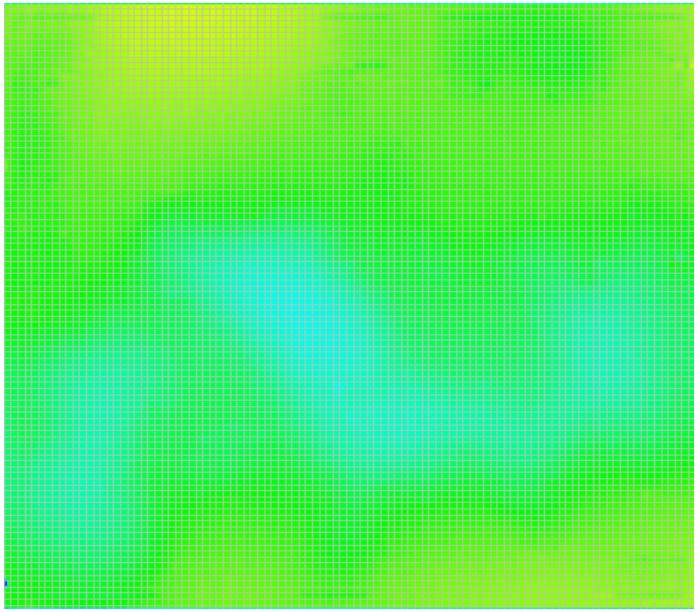


- Shock compression results in slightly higher mean temperature but hot spot temperatures are still ~800 K.
- Shock of samples with initially lower TMD (89%) leads to hot spots of ~850K

Influence of grain/grain friction

- We compared the behavior of SEM composite with different grain/grain friction and perfect interface (no-friction) case.
- The perfect interface case better represents intimate (partially reacted) interfaces between Al/Ni formed due to processing/preparation of SEM





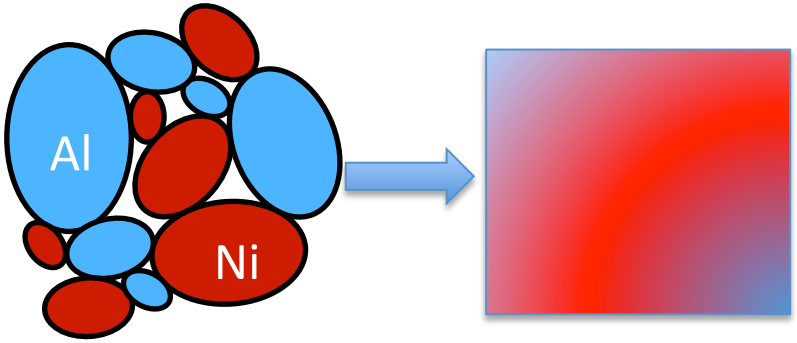
- In simulations with perfect interfaces the mean temperature is lower and the distribution is much more homogeneous (only 50K deviation from mean T) compared to simulations with friction

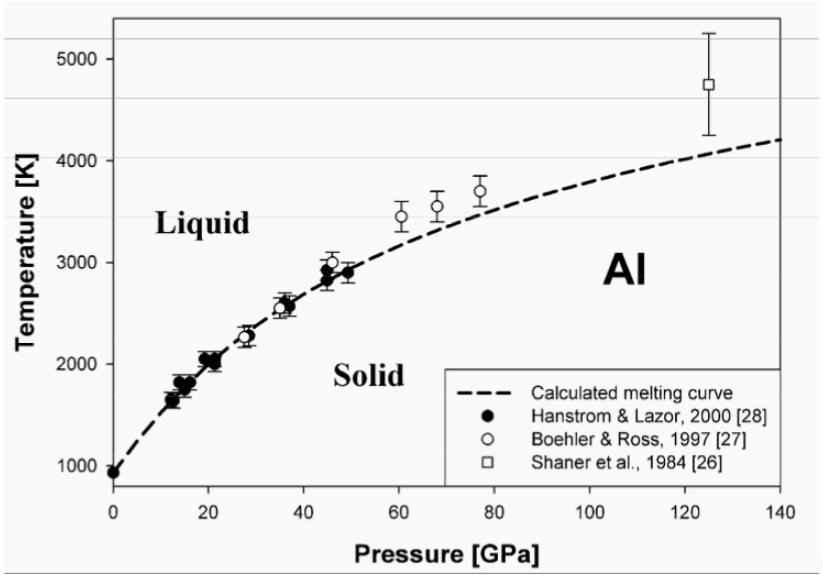
Key outcomes from mesoscale modeling of mechanical response of SEM materials:

- Homogenized Mie-Grueneisen EOS and linear hardening model have been obtained for composite material → will be used in *macroscale* simulations where microstructure is not resolved.

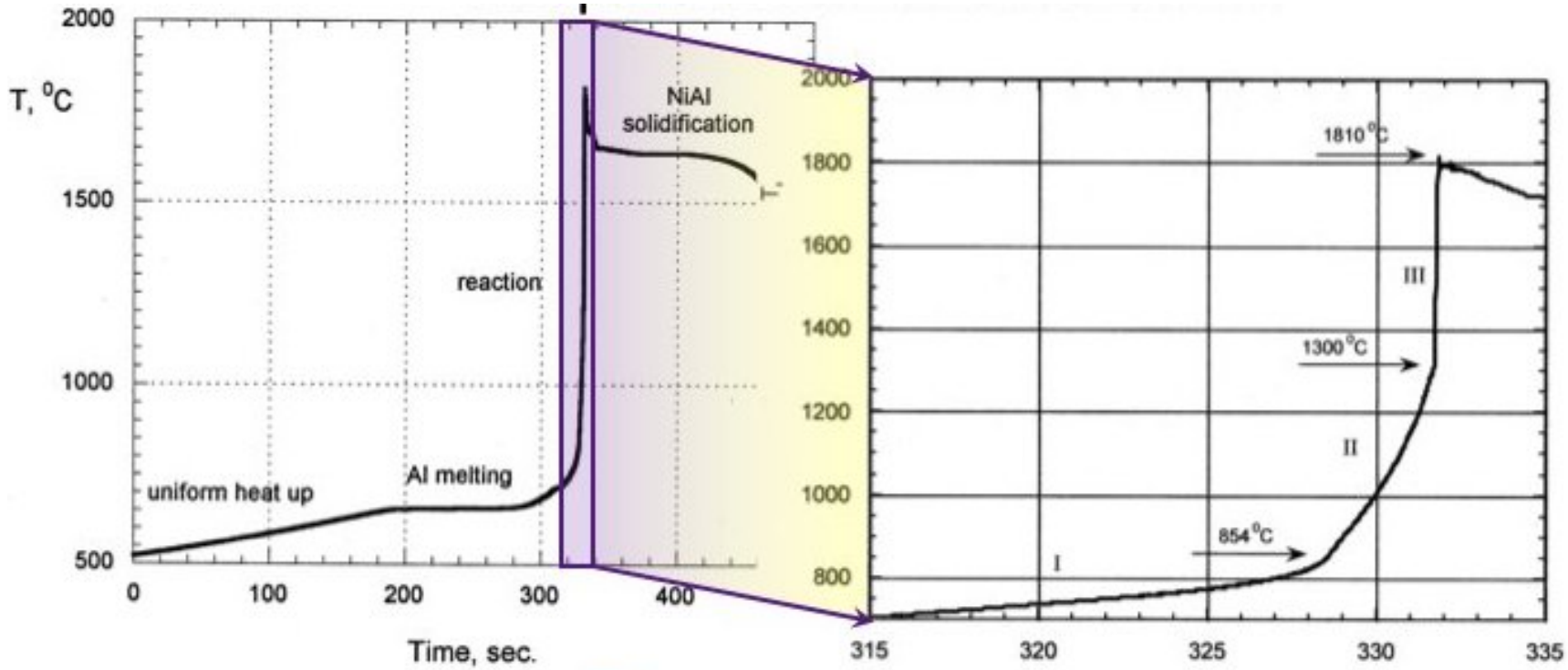
- Plastic deformations, mechanical work, and grain friction lead to modest increase of mean temperature and hot spots with T not higher than 800K.

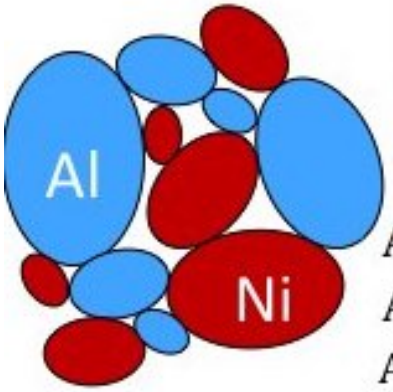
- Not sufficient to cause Al melting, particularly taking into account pressure dependence of T_m of Al

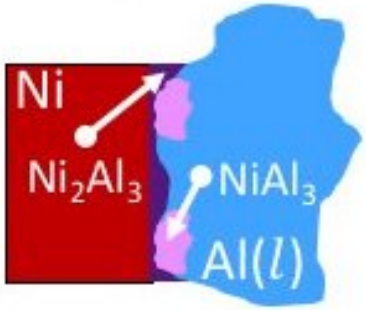


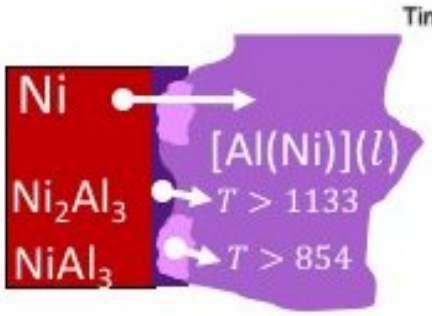


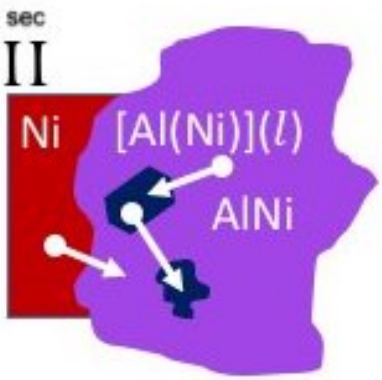
SEM reaction models in mesoscale MPM











$$Al(l) + Ni \rightarrow Ni_2Al_3$$
$$Al(l) + Ni \rightarrow NiAl_3$$
$$Al(l) + Ni \rightarrow Al(Ni)(l)$$

$$NiAl_3 \rightarrow Al(Ni)(l)$$
$$Ni_2Al_3 \rightarrow Al(Ni)(l)$$
$$Al(l) + Ni \rightarrow Al(Ni)(l)$$

$$[Al(Ni)](l) \rightarrow AlNi(l + s)$$

SEM reaction models in mesoscale MPM

In MPM code we have coupled the following phenomena:

- Thermal heat conduction
- Melting

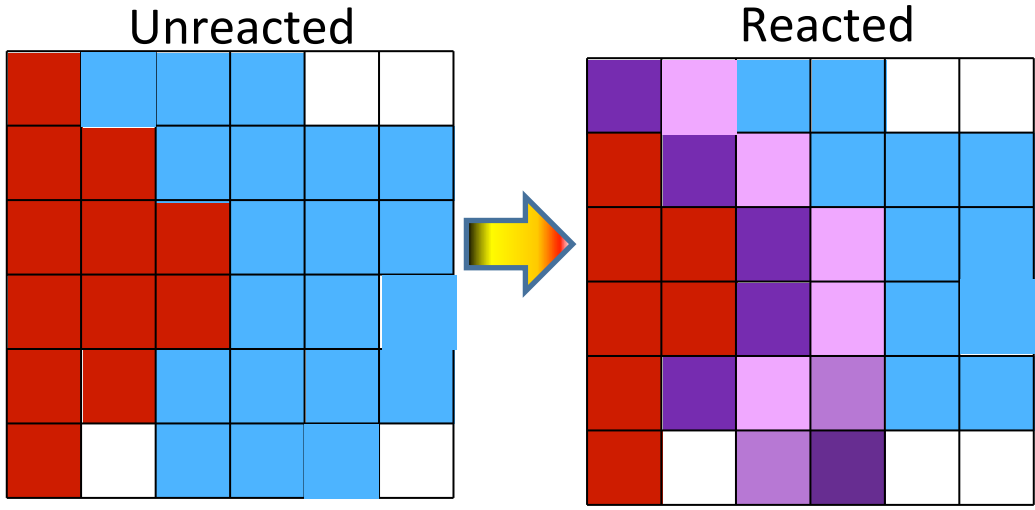
  Al(s)→Al(*l*), ΔH=10.7 kJ/mol

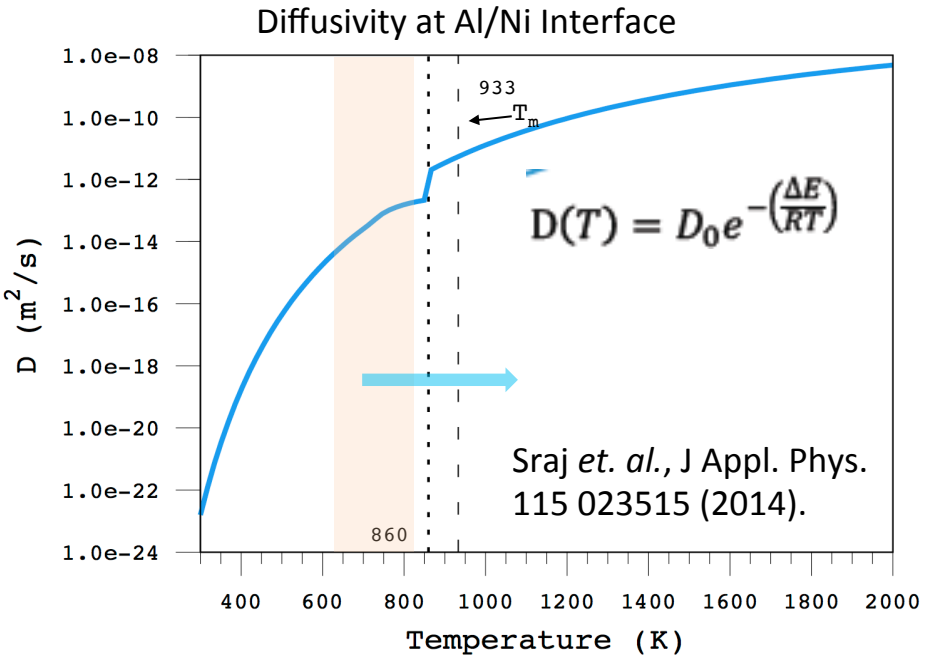
  Ni(s)→Ni(*l*), ΔH=17.5 kJ/mol
- Interdiffusion of species using temperature dependent diffusion coefficients
- Reactions

  currently all reaction steps are combined into one with

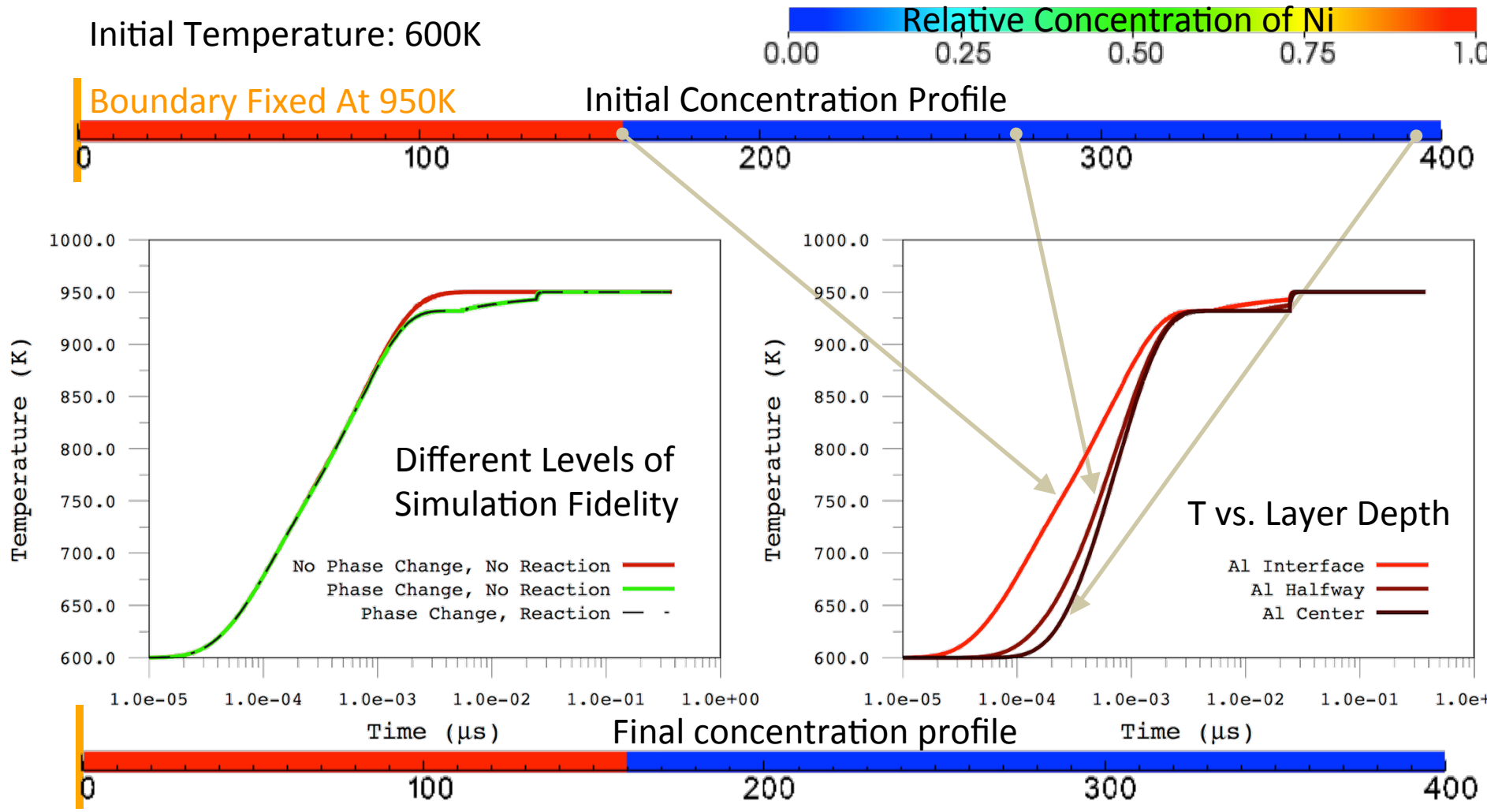
  ΔH = -152 kJ/mol

  (K. Morsi, *Mat. Sci. and Eng. A*, 299, 1-15)





Coupled reaction, diffusion, and thermal transport in mesoscale MPM

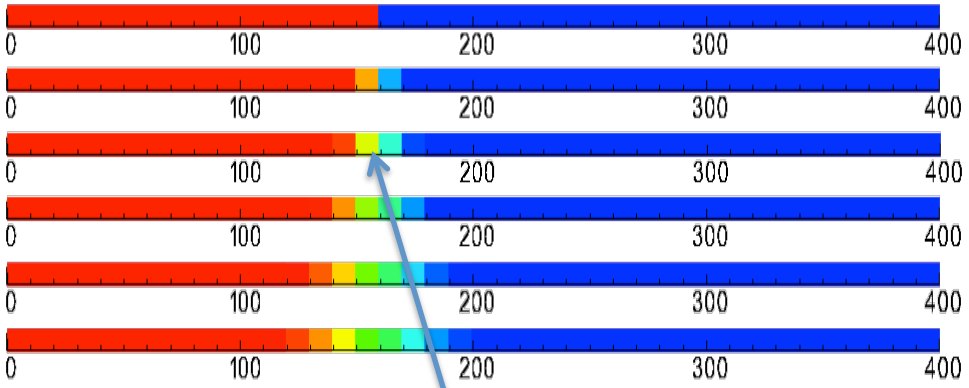


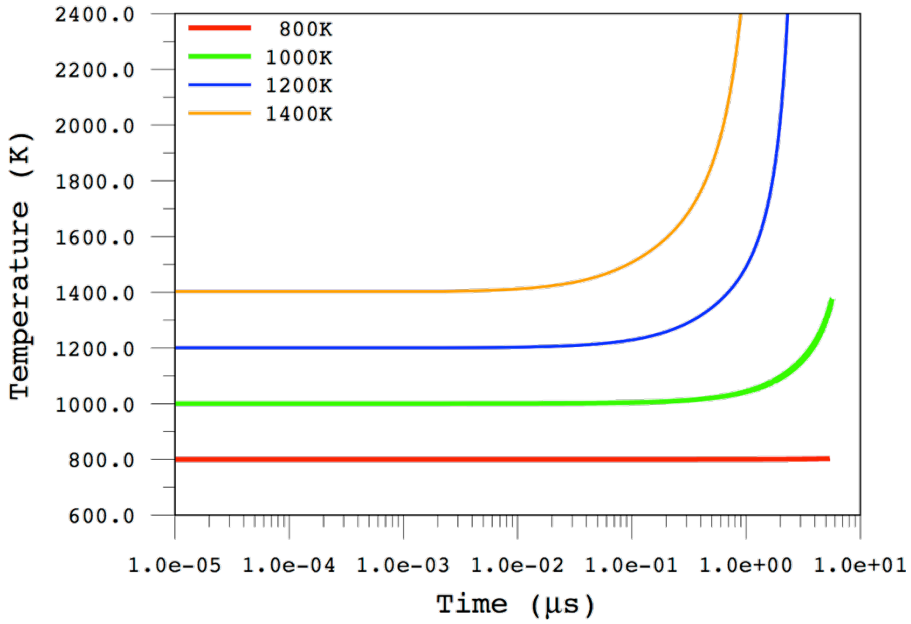
- No noticeable diffusion over temperature ramping time
- Thermal equilibration ‘instantaneous’; reaction is diffusion limited

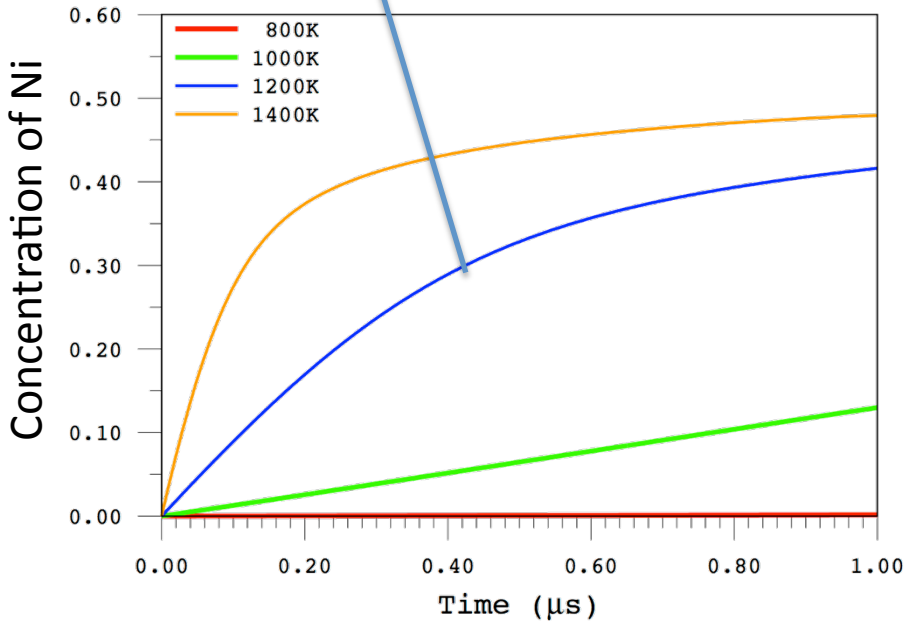
Coupled reaction, diffusion, and thermal transport in mesoscale MPM

Initial Conditions:

- Block of Ni in contact with Al
- Thermally insulated boundaries
- Initial T= 800,1000, 1200, 1400 K
- Temperature change purely from reaction







- At higher initial temperatures the diffusion is fast enough to result in substantial heat release and reaction front acceleration.

Key outcomes from mesoscale modeling of thermal transport, diffusion, phase transformations, and reactions in Al/Ni system:

- MPM simulation tool has been enhanced to couple interdiffusion, melting, reactions, and thermal dissipation. The code can handle arbitrary number of reactions (multiple stages) and transformations as well as temperature and material dependent parameters.

- At low temperatures (<600K) if we start with an interface of pure Al and Ni, the interdiffusion of Al/Ni is so slow that the heat generated due to reactions will be easily dissipated and insufficient to generate runaway reactions

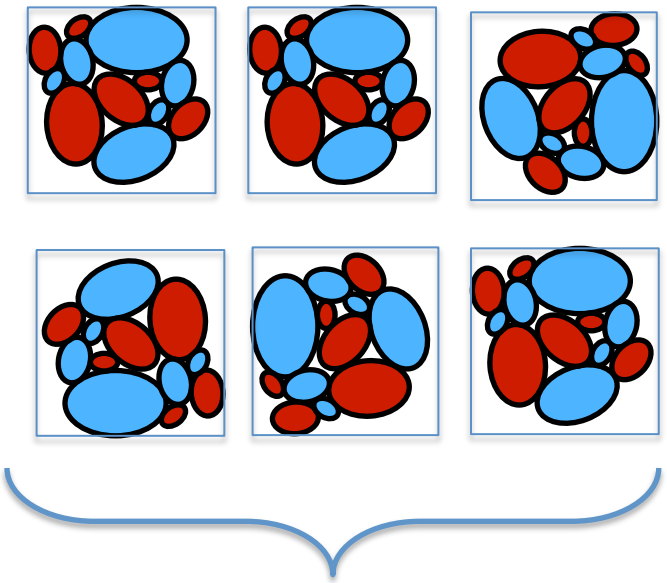
- Runaway reactions (on time scale of 100s of microseconds to several milliseconds) can be expected if the initial temperature of the material is >800K or some initial premixing at Al/Ni interfaces (but only partially reacted) occurred during SEM preparation.

- Note, these considerations do not take into account pressure effects on reactions and diffusion

Macroscale simulation of SEM container with PBX

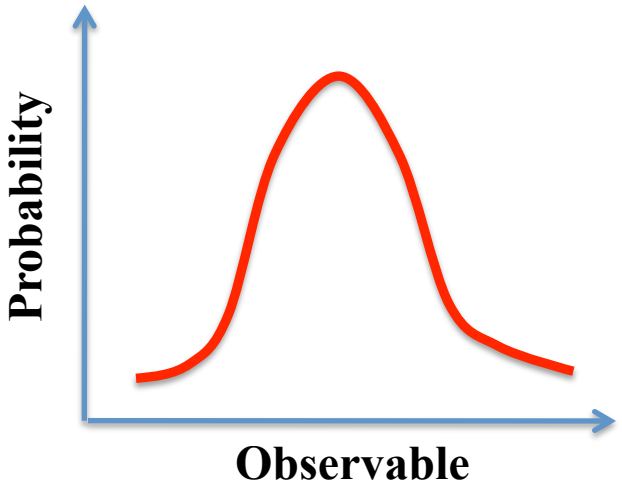
In these simulations we use:

- Homogenized properties of SEM obtained from sampling different configurations at mesoscale.
- Heterogeneous nature of SEM material properties is taken into account by stochastic distributions.



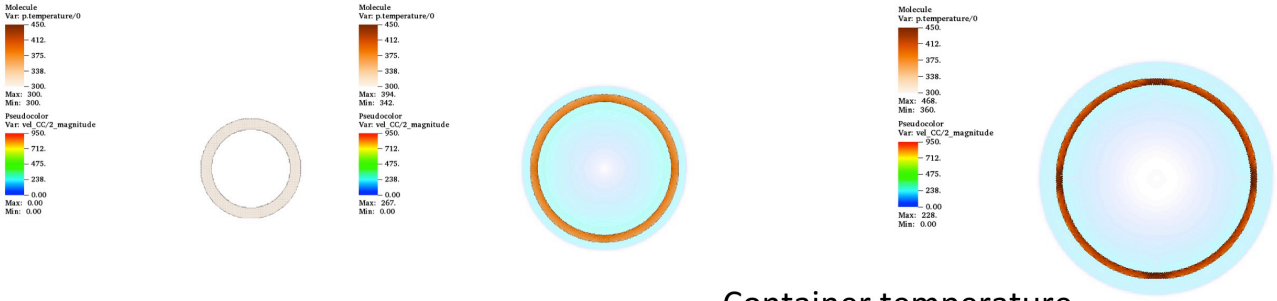
These simulations allow us:

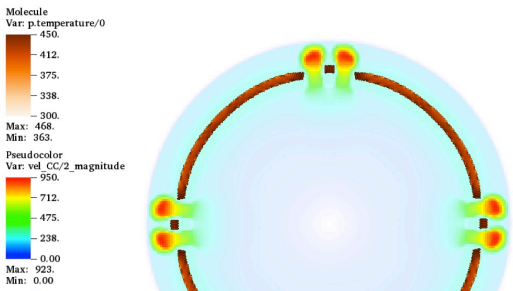
- To determine the relevant range of conditions (stress distribution, temperature, fragment velocity) which SEM material is experiencing.
- Establish correlations between molecular scale chemistry, mesoscale grain structure, failure mechanisms and the performance of the SEM-based device.



Homogenized engineering scale simulations (Macroscale MPM and MPM-ICE)

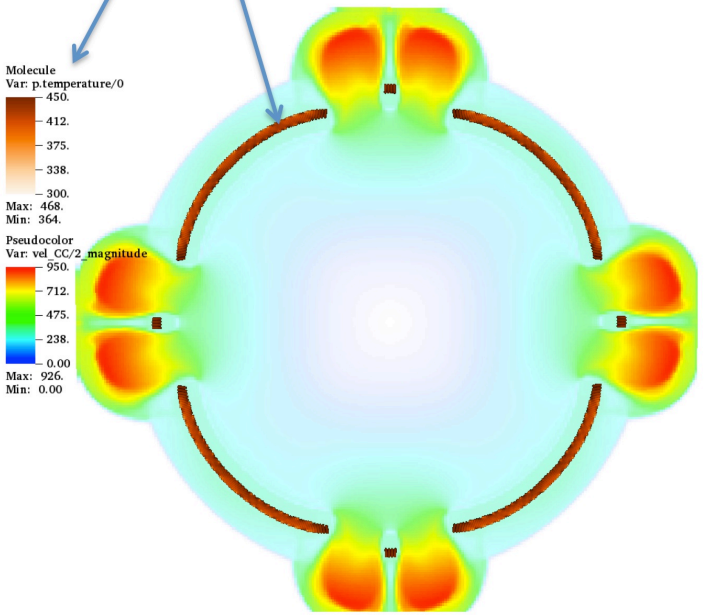
Explosion of PBX inside container with no heterogeneity in the container properties





PBX gas products velocity field

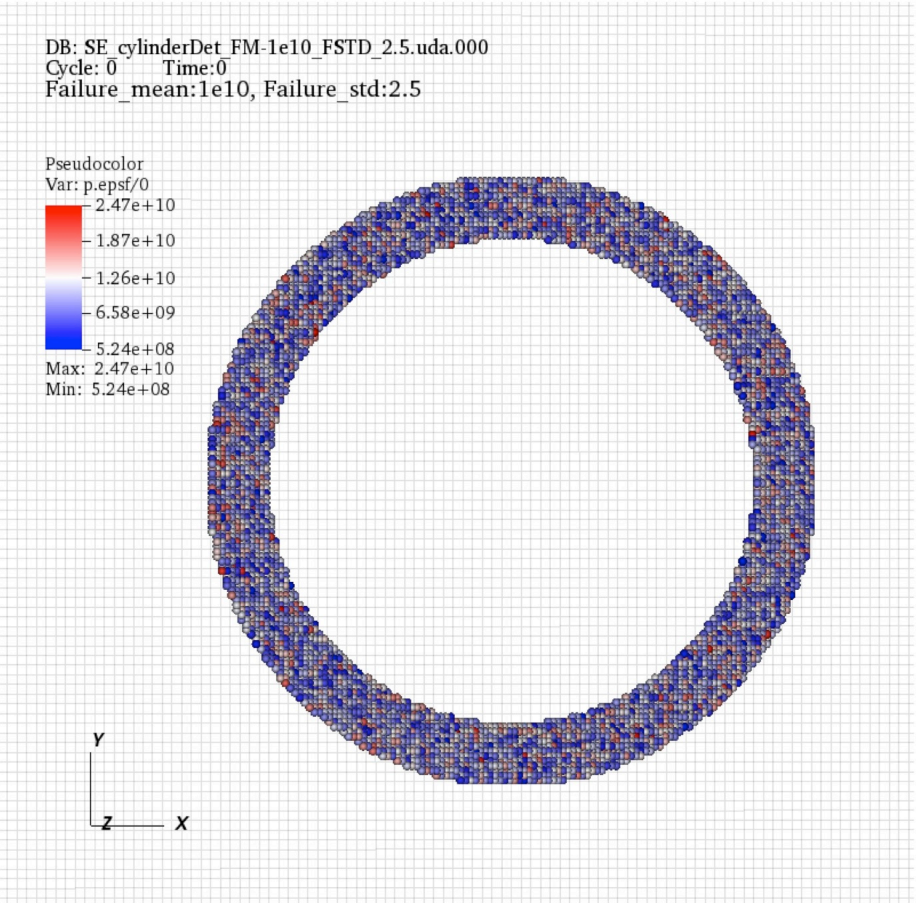
Container temperature field

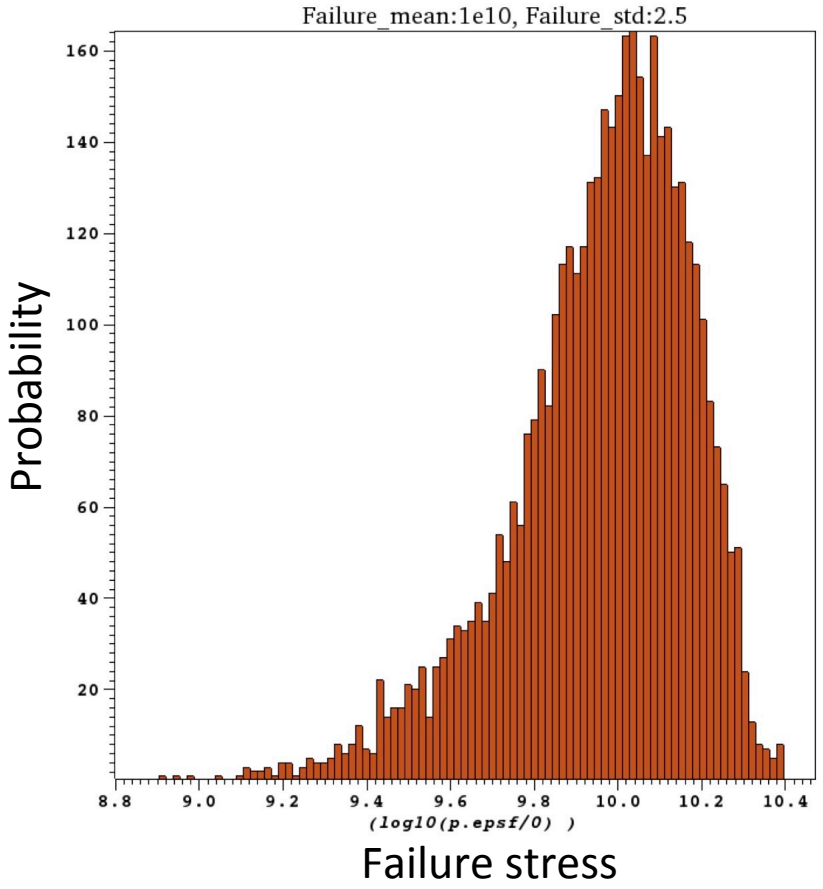


The container breaks into four large and symmetric pieces

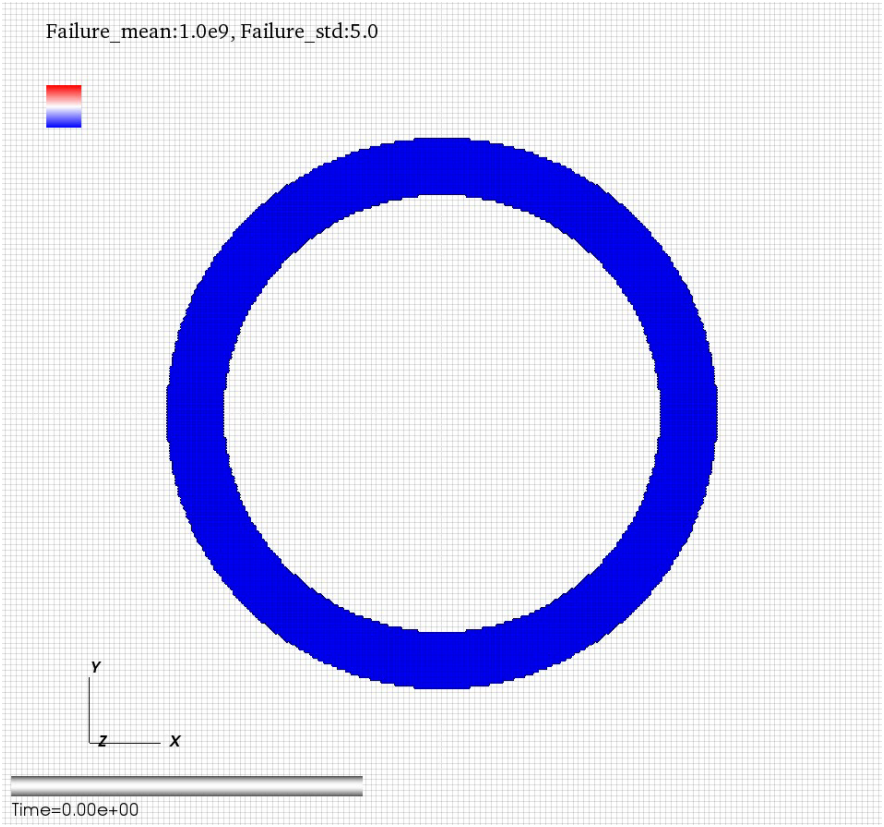
Homogenized engineering scale simulations with stochastic heterogeneity (Macroscale MPM and MPM-ICE)

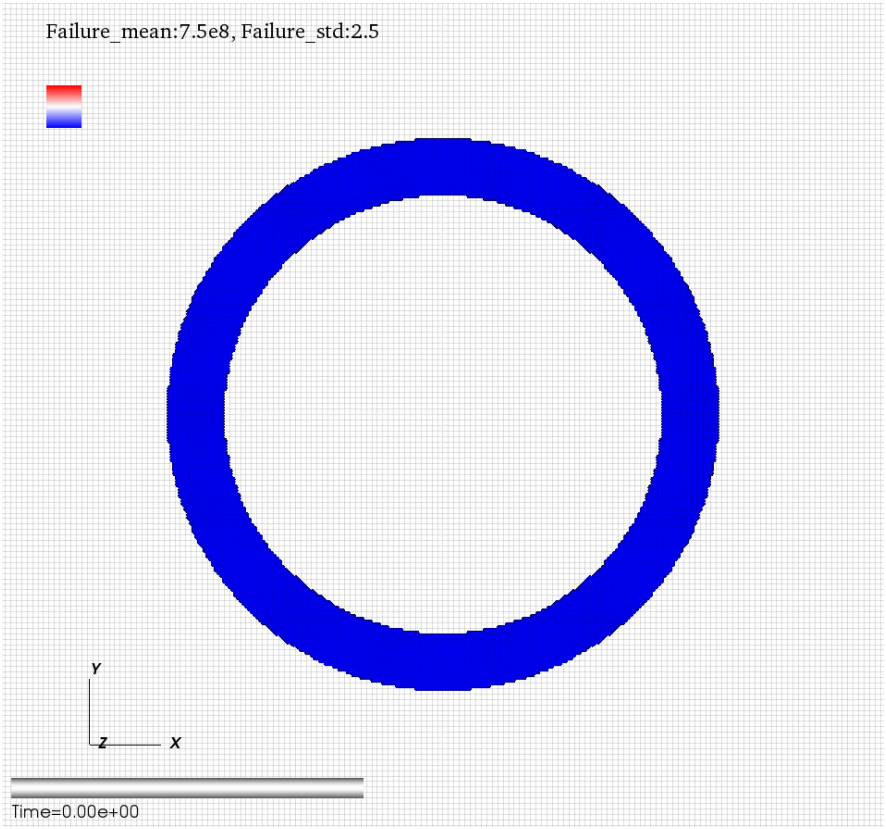
Now lets have simulation where the failure stress for each material point is taken from a stochastic distribution





Homogenized engineering scale simulations with stochastic heterogeneity (Macroscale MPM and MPM-ICE)

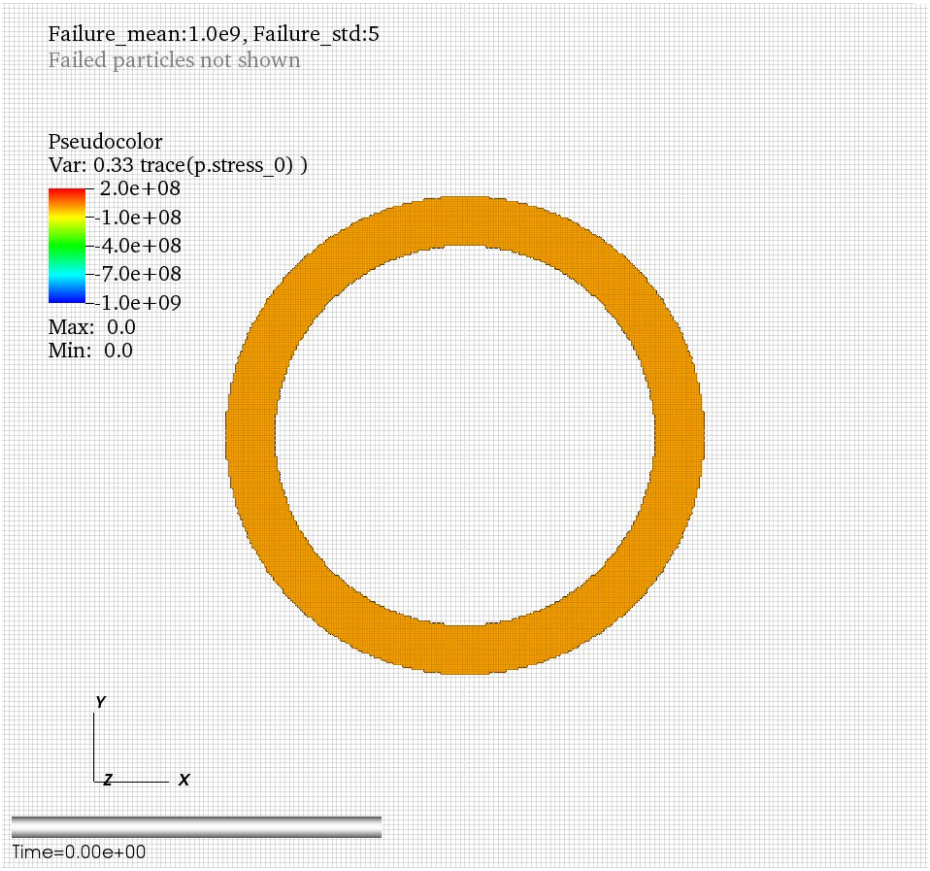




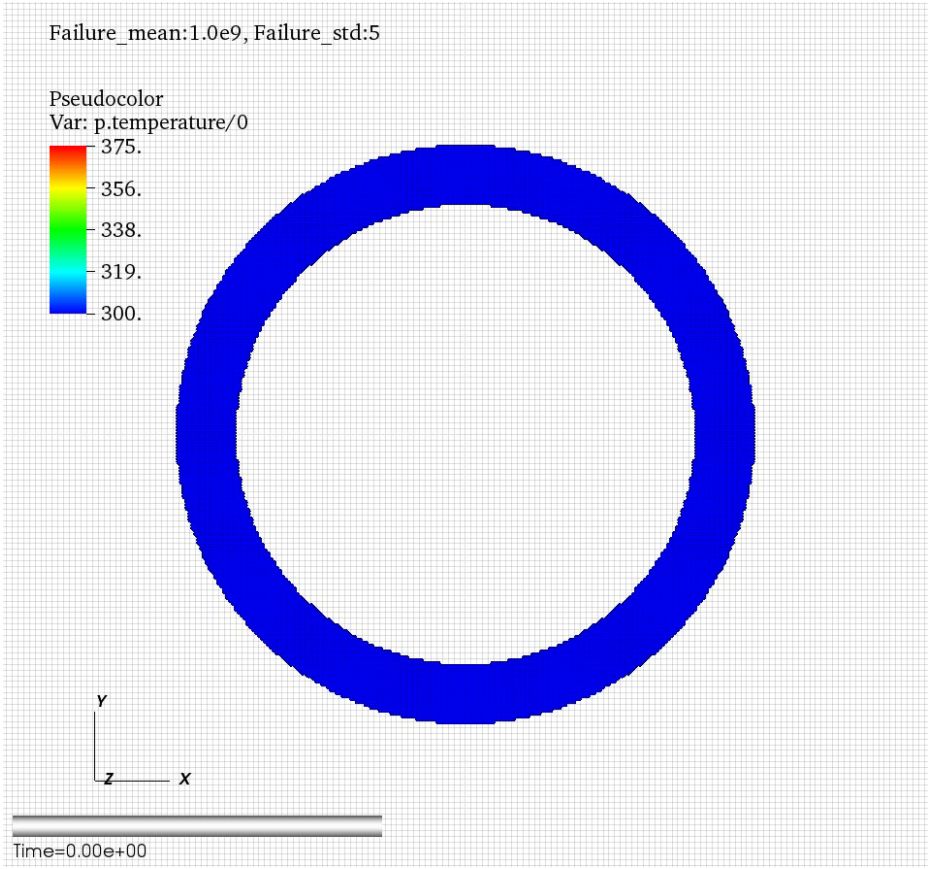
- Red points are “failed” points, i.e. points not supporting the stress
- Case on the left has large mean value and narrower distribution of failure criteria

Homogenized engineering scale simulations with stochastic heterogeneity (Macroscale MPM and MPM-ICE)

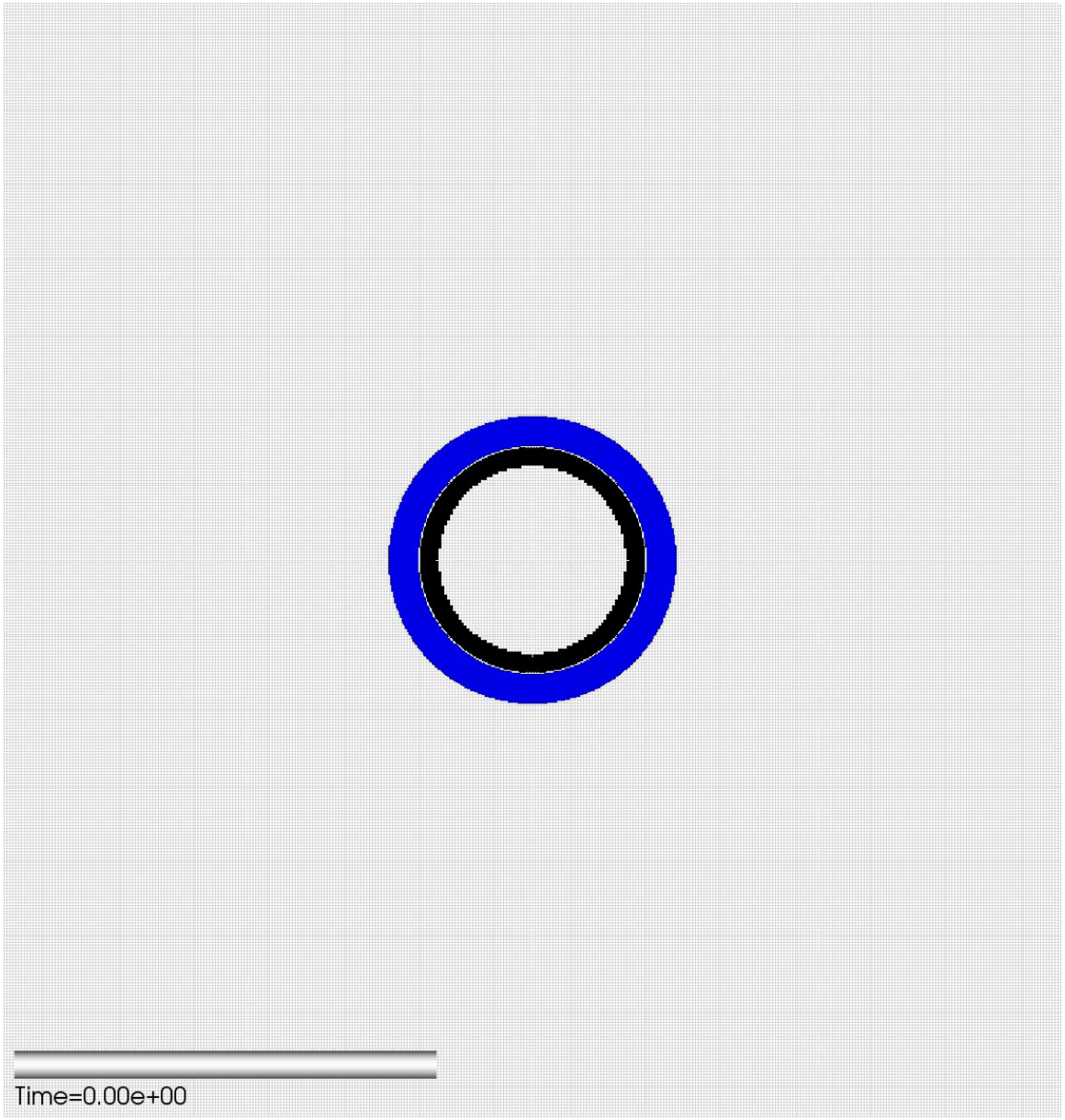
Stress distribution



Temperature distribution

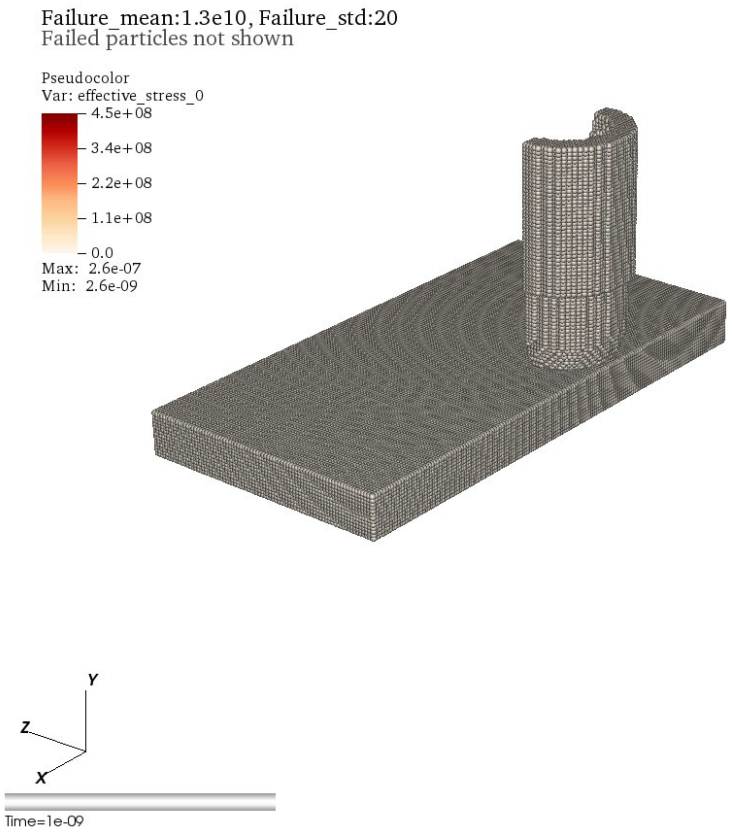


Homogenized engineering scale simulations with stochastic heterogeneity (Macroscale MPM and MPM-ICE)

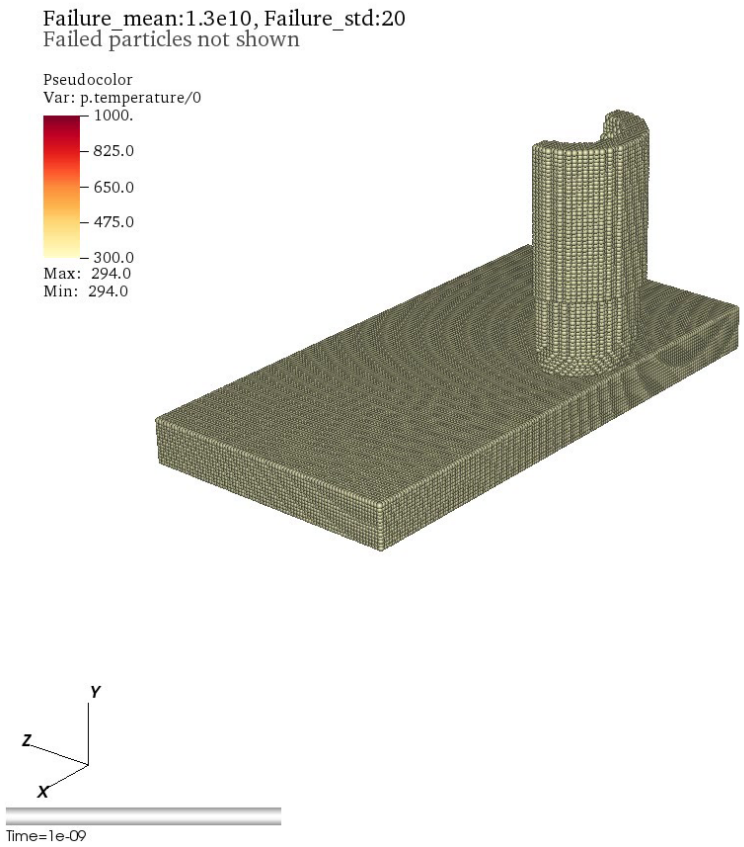


Tracking fragments and their impact (Macroscale MPM-ICE)

Stress distribution



Temperature distribution



- By the time of impact (hundreds of microseconds or milliseconds) the SEM fragment can generate significant heat due reactions
- Upon impact the fragment kinetic energy converts into thermal energy which can further boost ongoing reactions in SEM

Key outcomes from macroscale simulations

- The material models and constitutive properties for these macroscale simulations come from atomistic/mesoscale simulations.

- These simulations allow to determine key time scales and distribution of conditions/environments experienced by the SEM materials during insult scenario.

- Include fluid/solid structure coupling. Are capable to deal with large deformations and multimaterial representation.

- Allow to establish correlations/dependence between atomic scale reaction mechanisms, mesoscale microstructure of SEM, and the engineering scale device performance.

Moving forward to Phase II

Key issues to address:

- **Enhance reaction model description**
- **Enhance damage/failure models**
- **Take into account the role of initial SEM processing**
- **Efficient coupling of phenomena with different time scales**

Role of processing

- Our simulations demonstrate that shock loading of high density SEMs (e.g., 90% + TMD) does not lead to reaction (e.g., hot spots are not sufficiently hot)

- However, reactions are observed experimentally in many Al/Ni composites:

  Shock loading (> 15 GPa) of low density (e.g., 50-60% TMD) materials with nanosized grains

  - A lot of frictional heating
  - A lot of interfaces, relatively little “bulk” material

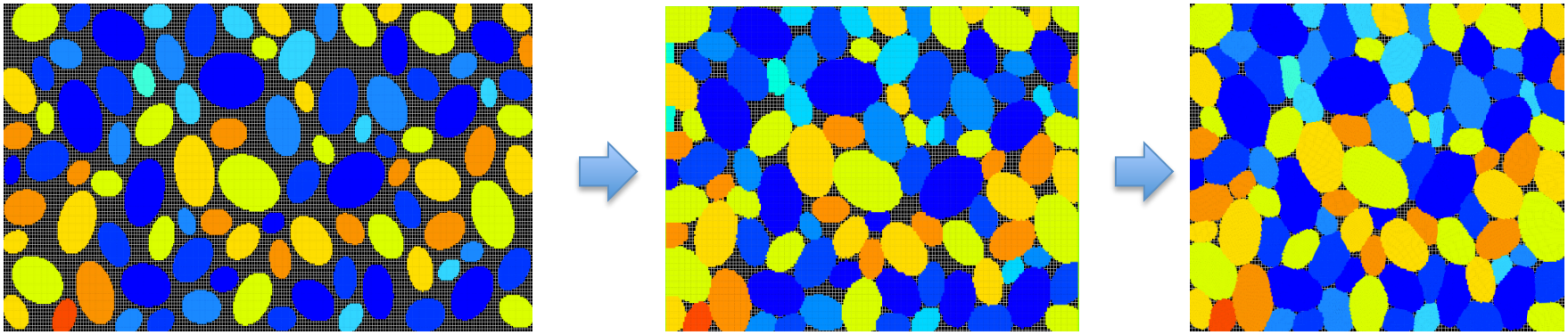
  Shock loading (> 15 Gpa) of high density SEM materials (granular and multilayer) that have experienced specific processing conditions

  - Shock loading (< 15 GPa)
  - Hot isostatic pressing (800 K +, several GPa ?)
  - High shear
  - Reactive milling

Role of processing

Where does the difference lie?

- Our simulations have emulated hot isostatic pressing, but do not include changes in the Al/Ni interface that might occur during processing



Al/Ni composite at 60%, 89% and 96% TMD from MPM simulations

- It is known that the Al/Ni interfaces transform during processing
  - resulting SEMs have good mechanical integrity
  - experimental analysis of post-detonation fragments indicate that the failure does not occur preferentially at the grain/grain boundaries

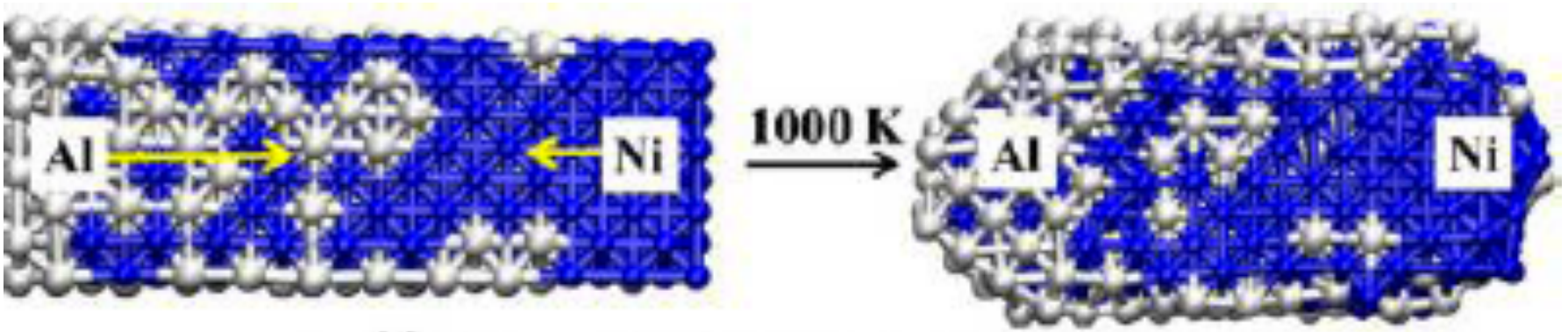
Role of processing

How Processing Influences SEM Reactivity?

- Diffuse/partially reacted (intimate) Al/Ni interfaces are indicated
- Our preliminary simulations indicate that such interfaces are much more susceptible to further reaction than pristine, sharp interfaces
- In Phase II we will include diffusion/reaction effects in mesoscale MPM simulations of processing
  - Informed by atomistic simulations
  - Shock loading
  - Hot isostatic compression
  - Other
  - Influence on performance and optimization

Enhancement of reaction/diffusion models: Atomistic Simulations

- EAM (embedded atom method) and/or ReaxFF will be used
- Both have been used to study Al/Ni interfaces and reactions
- No studies of the influence of ***pressure*** on diffusion and reaction have been performed



Enhancement of reaction/diffusion models: Atomistic Simulations

- MD simulations will play a key role in Phase II:
  - Quantify the influence of pressure on Al/Ni interdiffusion
  - Quantify the influence of pressure on Al/Ni reaction (mechanisms and heats of reaction)
  - Understand the nature of the Al/Ni interface, including structure, strength and fracture toughness
  - Influence of pressure on Al melting T at Al/Ni interface

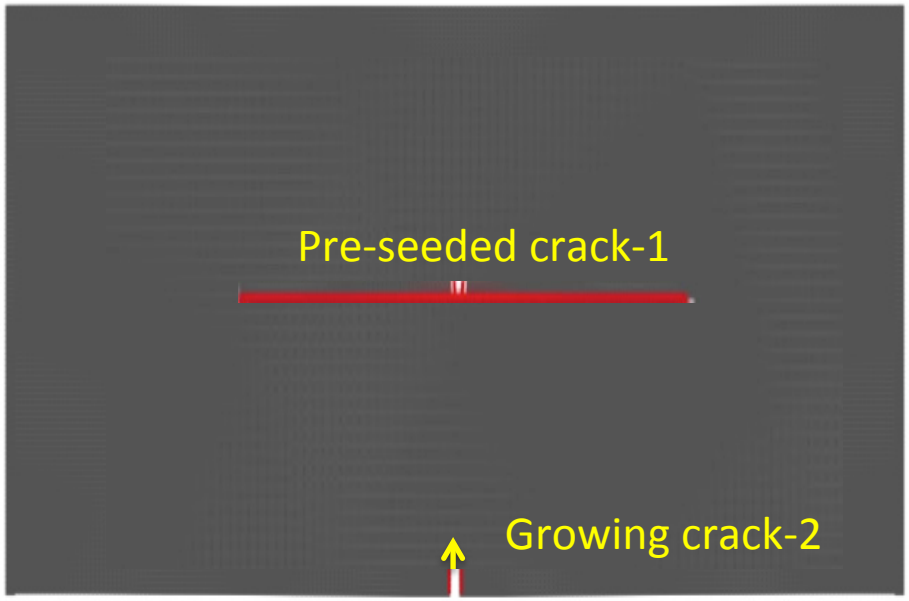
Enhancement of failure models: Damage Mechanics

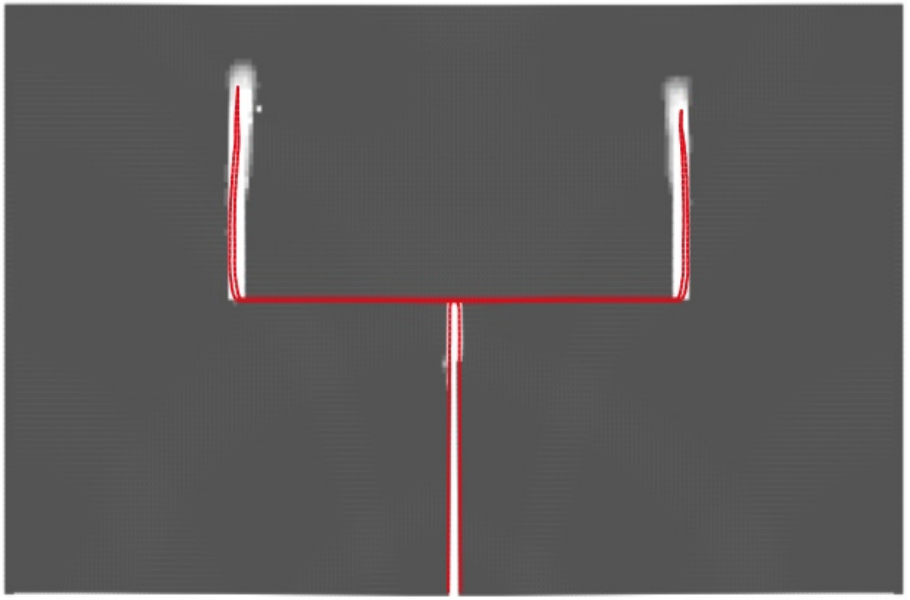
- The team will be enhanced by Pro. Nairn (Oregon State University) who is world expert in modeling of damage mechanics.
- Damage mechanics has been developed as an alternative method for modeling damage evolution in complex materials.
- In brief, damage mechanics replaces displacement discontinuities of explicit cracks with altered constitutive laws for the material.
- Despite the attraction of damage mechanics models, the vast majority of implementations have a major drawback in that they resort to the special case of "isotropic" damage.
- We claim that isotropic damage mechanics are inadequate. In contrast, our new methods include anisotropy and we have demonstrated a rigorous connection to fracture mechanics
- When materials develop damage and cracks, **they become anisotropic**.

Enhancement of failure models: Damage Mechanics

- Our claim is that it is vitally important that any numerical modeling approach to predicting cracks (*e.g.*, damage mechanics) must demonstrate that it can reproduce explicit crack results when applied to the same problem.

- Furthermore, this comparison/validation allows for parameterization of the ADaMM based upon fracture mechanics properties.





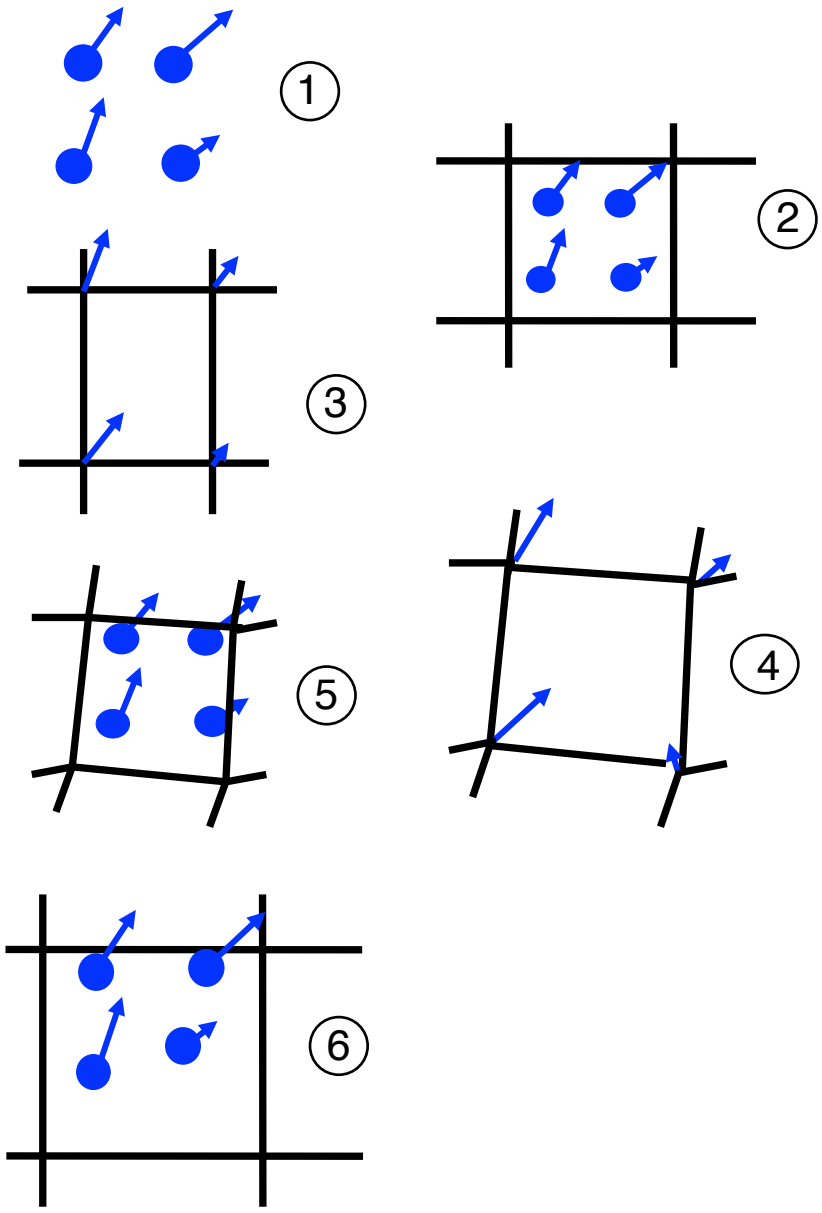
Superposed crack path results from an explicit crack model (red line) and a damage mechanics model (particles in white).

Open questions and desired input from the Air Force:

- Should we work with model microstructures (as in Phase-I) or Air Force plans to provide specific SEM microstructures for Phase II?
- Are there any fracture measurements/data for existing SEMs?
- Can we get information on specific processing conditions that are typically considered to make SEMs with high % TMD?
- Are their specific device performance characteristics that should be taken into account (e.g., fragments size distribution, flying time, impact properties, etc.)?
- Is Air Force interested in using our simulation tools or should we focus on the development of more generic physics-based models that can be subsequently implemented into other codes?

Thank you!

Multiscale Modeling Approach: MPM



Material Point Method **-** is a mixed grid /particle method

1.Particles with properties (velocity, mass, etc)

2.Defined on a mesh

3.Particle properties mapped onto mesh points

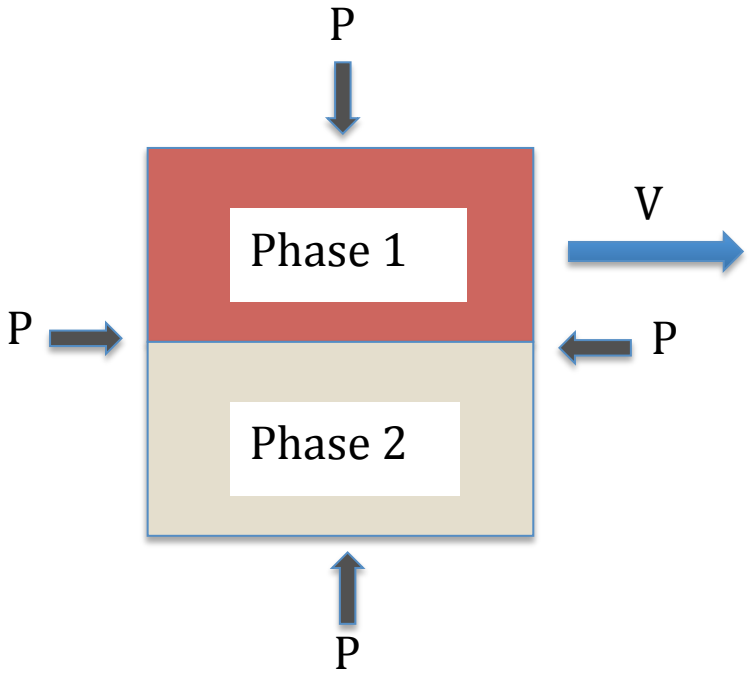
4. Forces, accelerations, velocities calculated on mesh points

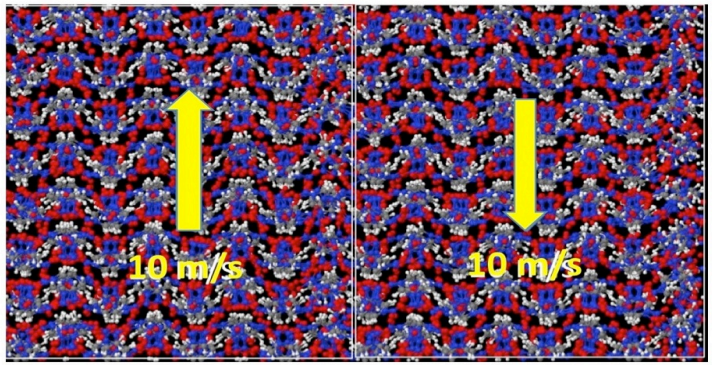
5. Mesh point motion calculated.

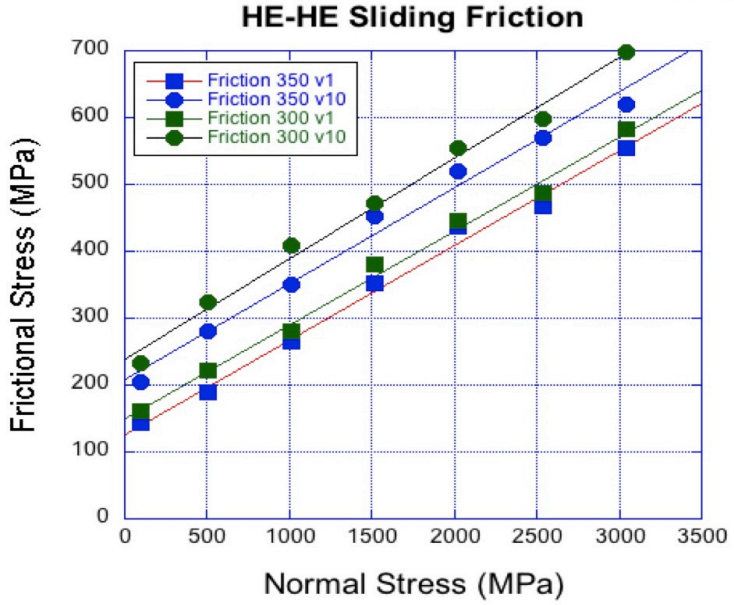
6. Only the particles moved by mapping velocities back to particles

Parameters for Al-Ni friction model

- Friction models for Al/Al, Ni/Ni and Al/Ni from atomistic MD simulations using Embedded Atom Model (EAM)







Phase 1 = Al or Ni

Phase 2 = Al or Ni

P = normal load (0 to 5 GPa)

V = sliding velocity (1 m/s to 10 m/s)

T = 300 K to 900 K