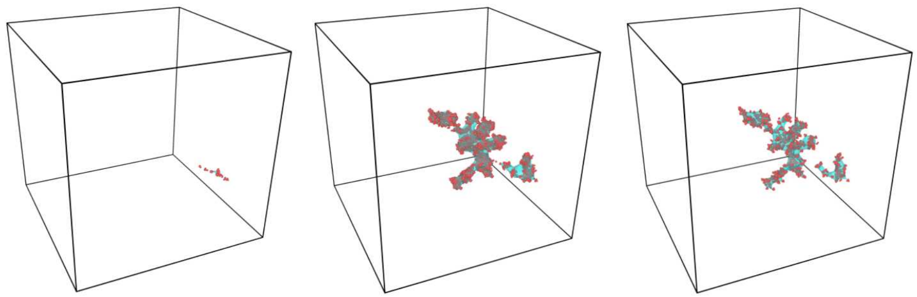
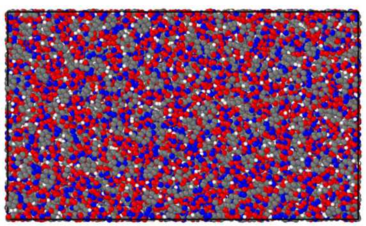
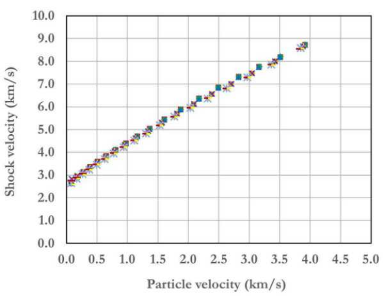
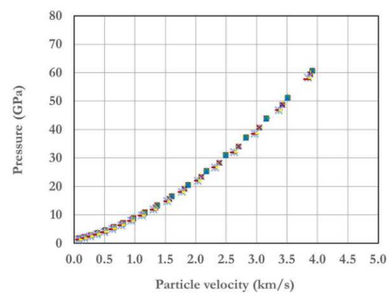
SAND2019-15020PE

Atomistic Insights of Materials in Extreme Environments via Virtual Characterization









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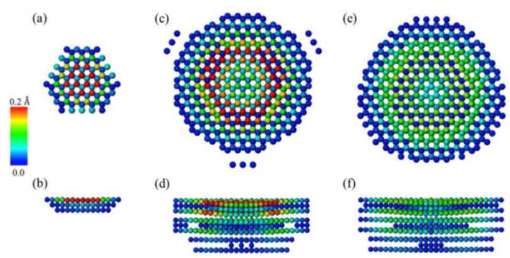
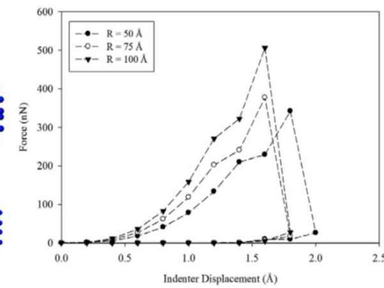
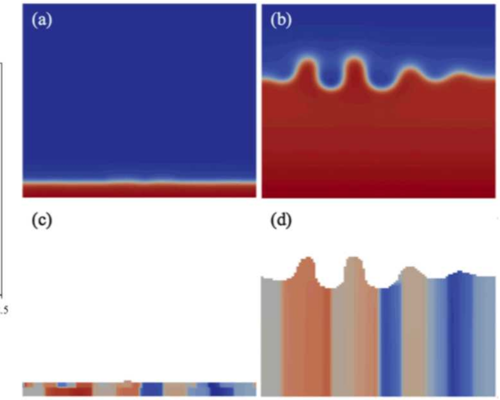
Summary of background

M.S. & Ph.D., Applied Physics

- Research focus: Atomistic modeling of nanoindentation on MoS_2
- Research focus: Phase-field modeling for PVD of polycrystalline materials

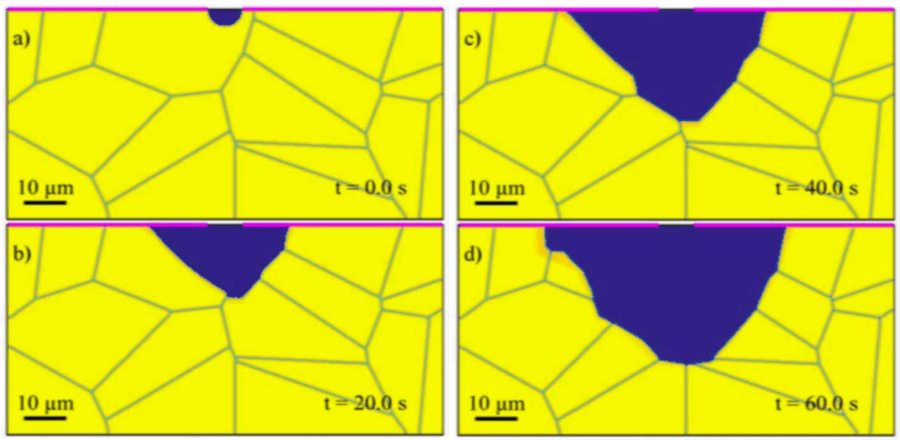


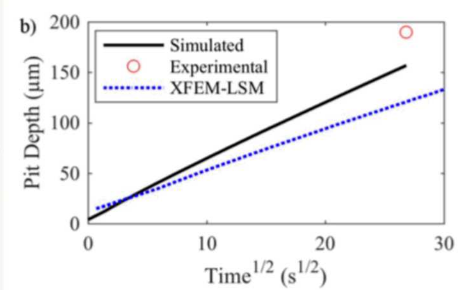




Research Fellow, Department of Materials Science & Engineering

- Research focus: Microstructural influences on localized corrosion in alloys

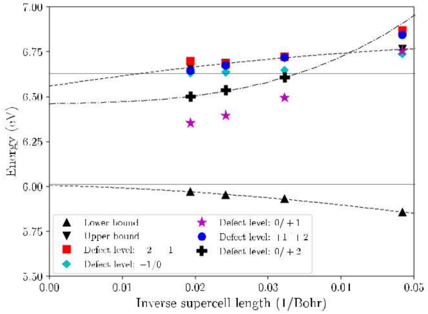


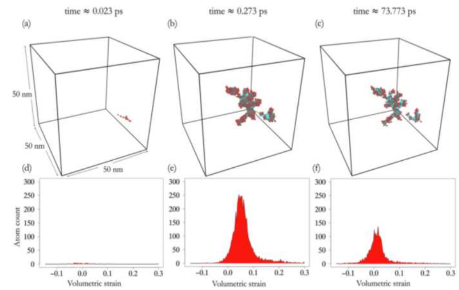


Summary of background

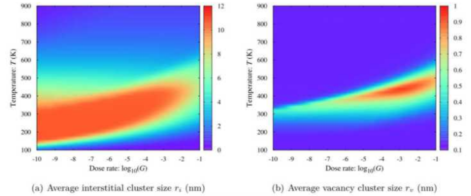
Postdoctoral Appointee, Nanostructure Physics Department

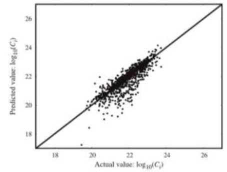
- DFT and MD modeling of radiation damage and shock loading

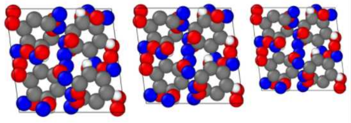


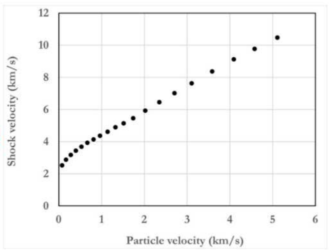


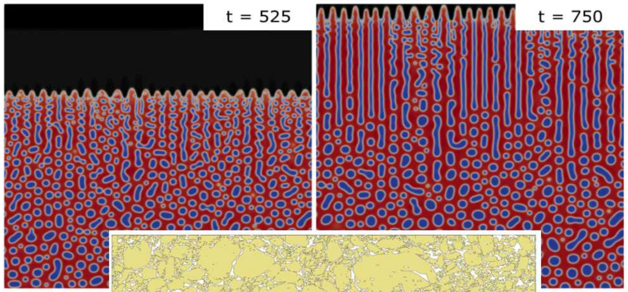
- Mesoscale modeling for radiation tolerant nanostructures and shock properties of energetic materials

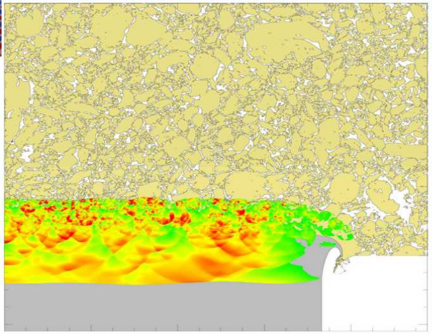












Topics to be covered

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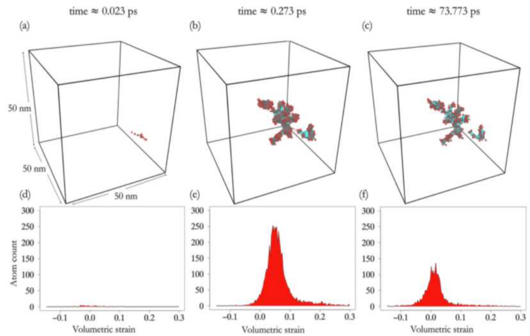
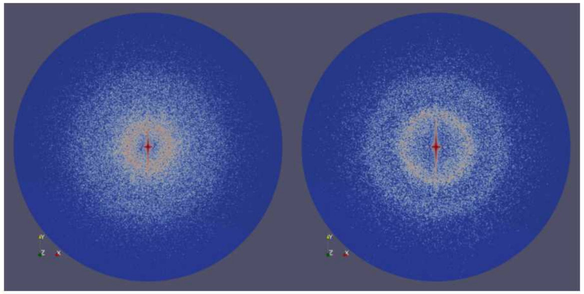
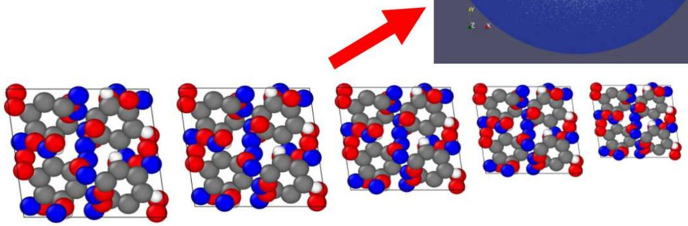
1. **Radiation Damage:** Characterizing displacement cascade damage in bulk silicon via virtual diffraction
   - Simple picture of single ion strike
   - Experimental (dis)connection
   - MD simulation and characterization



2. **Shock Behavior:** Gaining insights on the role of crystal structure on shock Hugoniot relations for HNAB via MD
   - Current experiments and related needs
   - Unreacted Hugoniots via MD
   - Virtual characterization

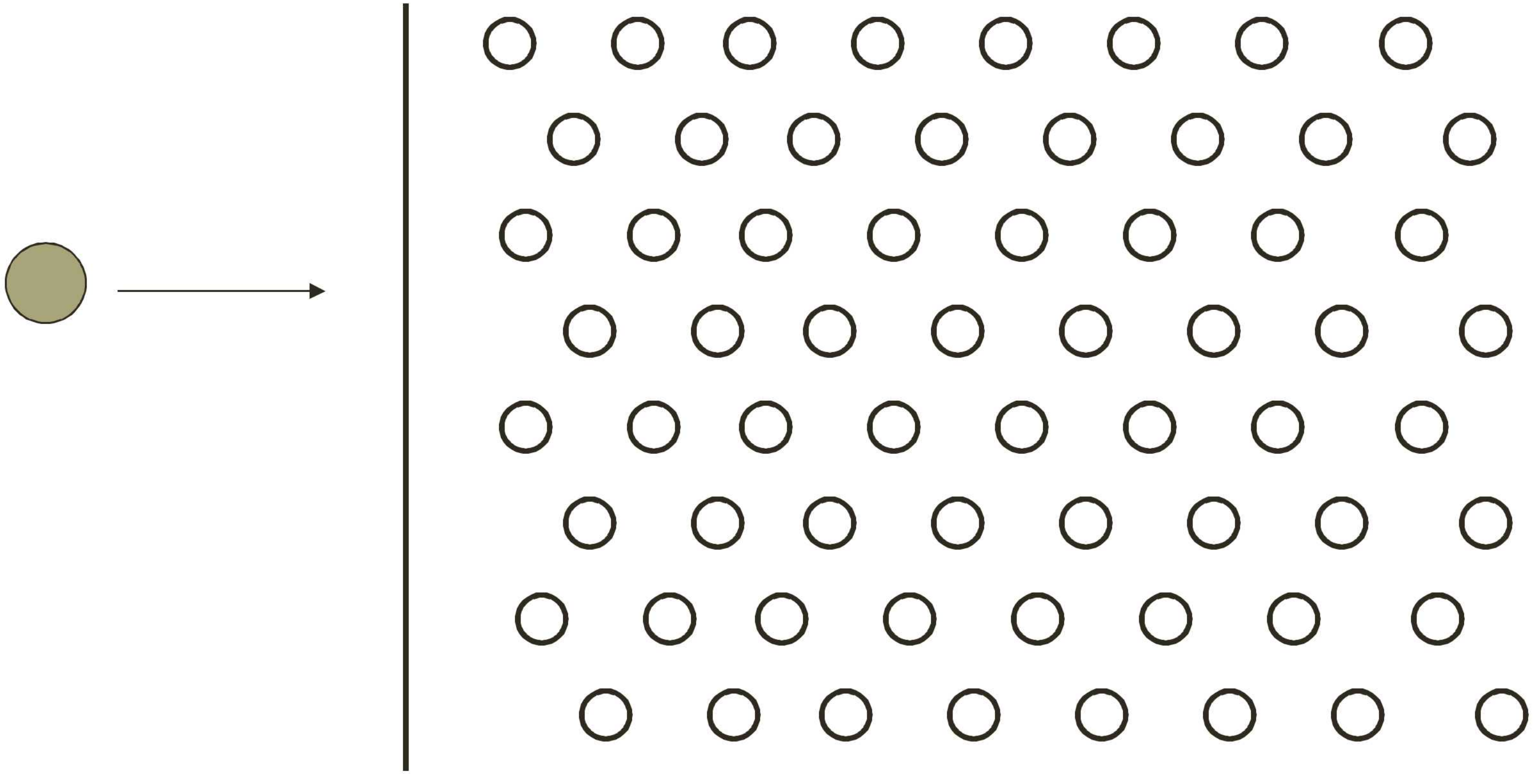




Example 1: Radiation Damage

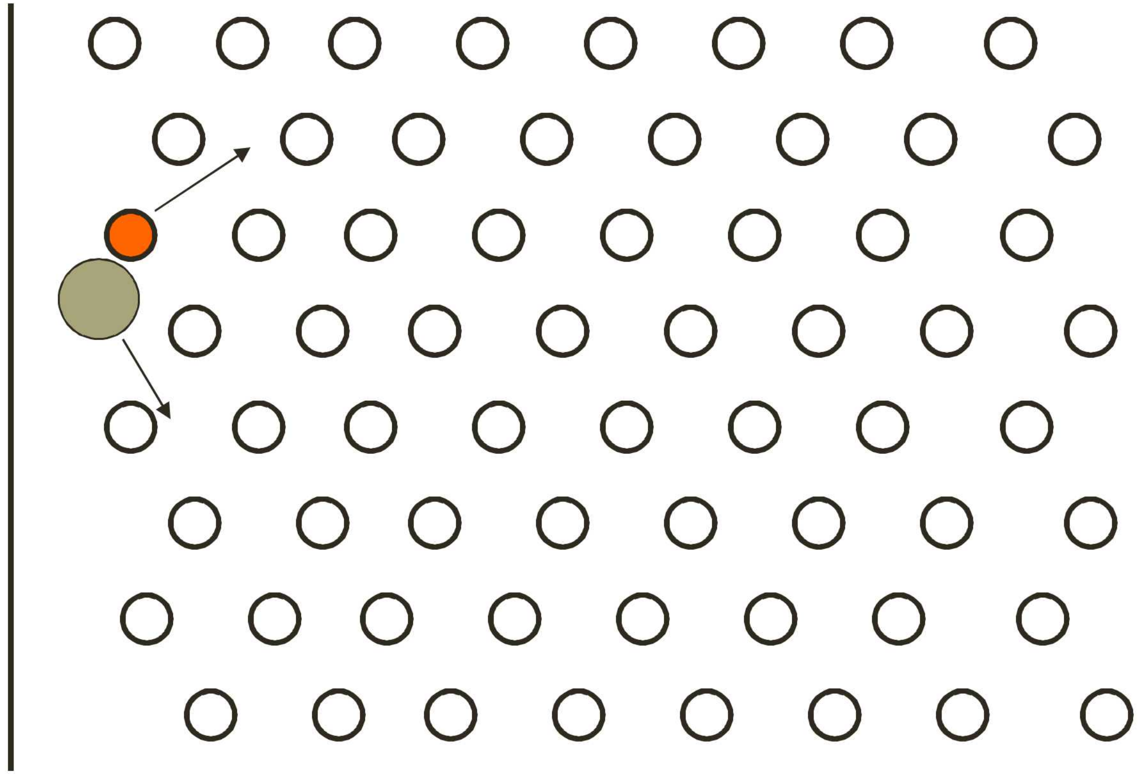
Characterizing Displacement Cascade Damage in Bulk Silicon via Virtual Diffraction

Simple picture: Incident energetic particle



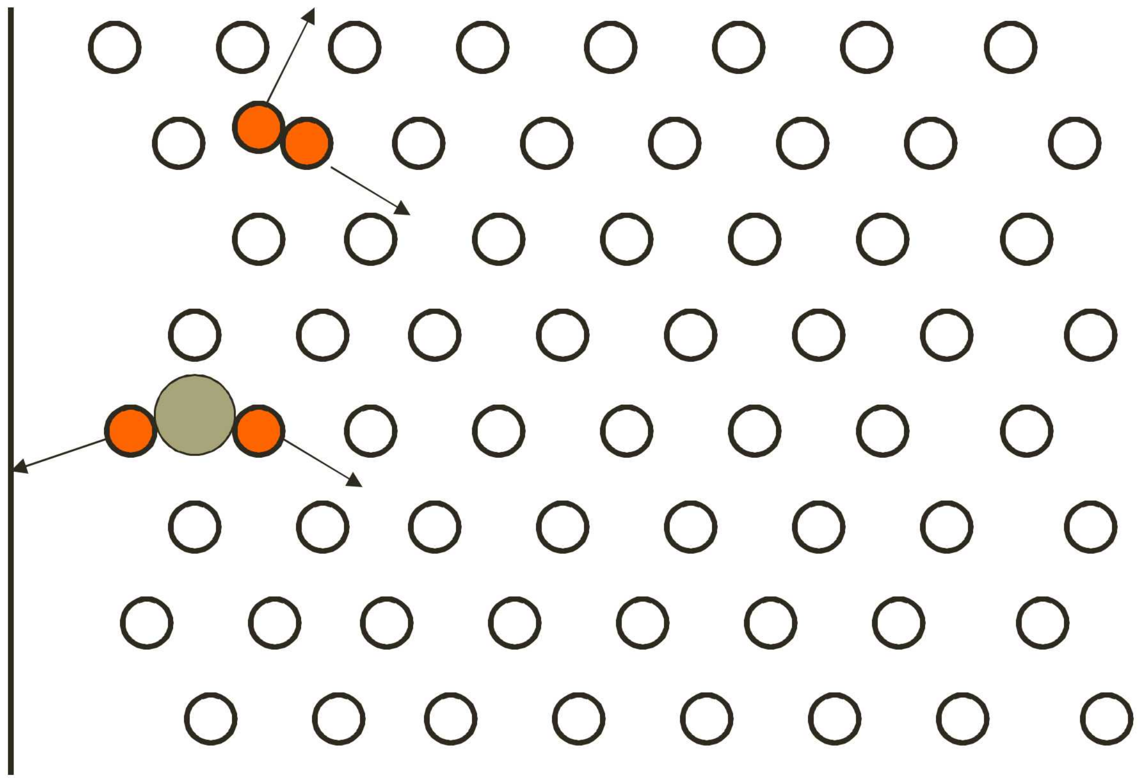
- **Energetic particle:**
  - Electron, neutron, ion (light/heavy)
  - Initial kinetic energy, incoming angle, neutral vs. charged particle

Simple picture: Transfer of energy to lattice atom



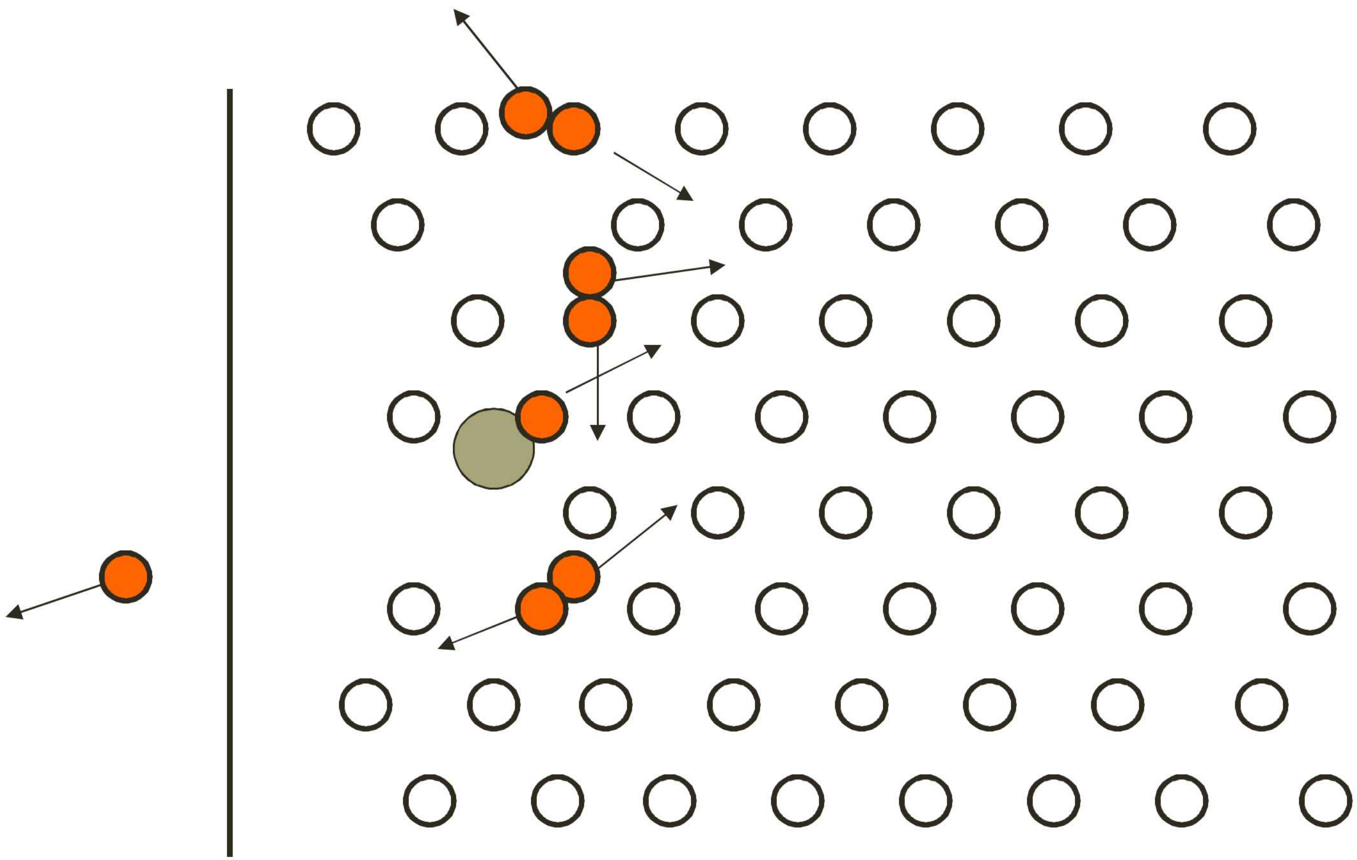
- **Primary knock-on-atom (PKA):**
  - Threshold displacement energy
  - Elastic and inelastic collisions, type of interaction, ionization

Simple picture: PKA moves from its lattice site



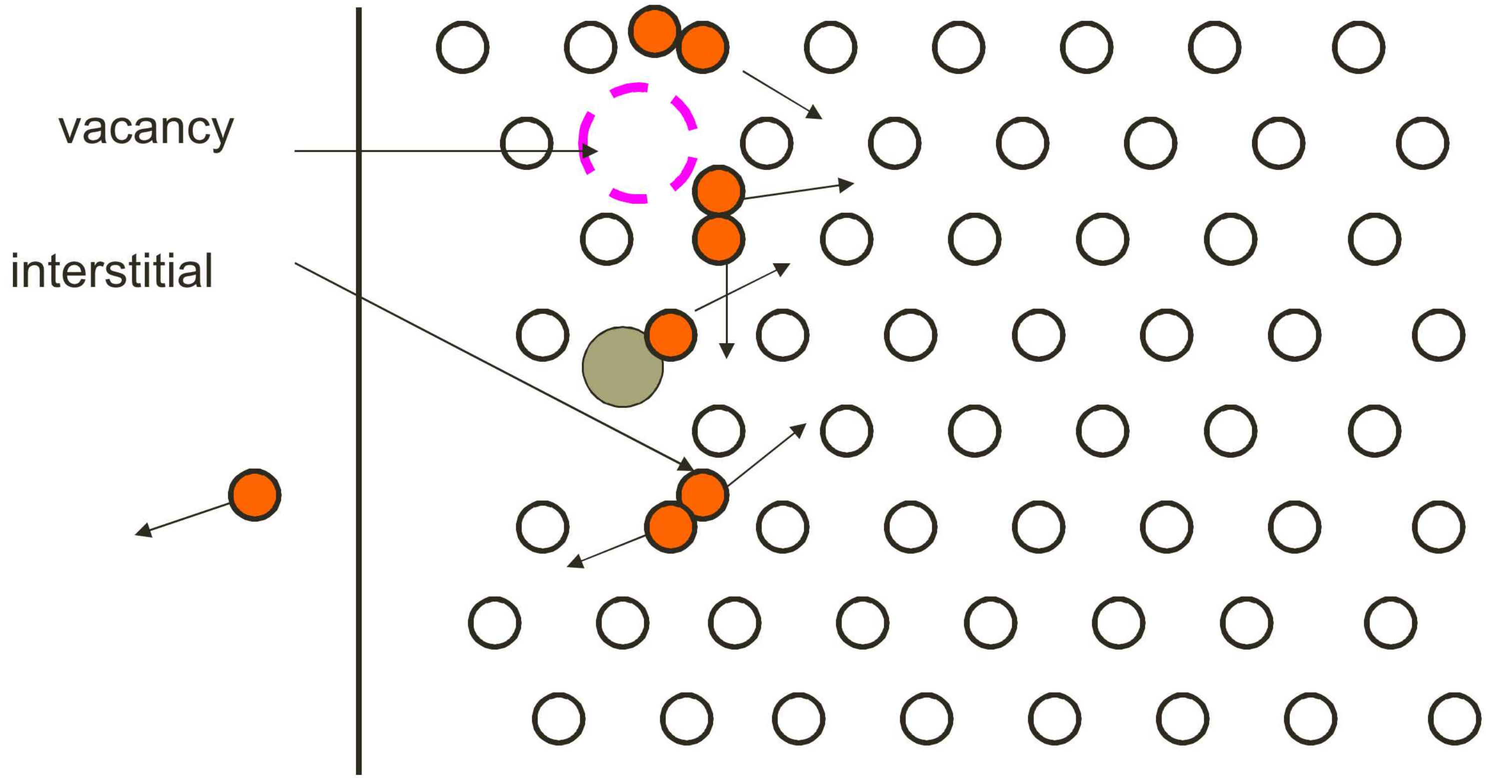
- **Secondary knock on:**
  - Lattice atom displaced by PKA
  - Slow down process: electronic stopping, nuclei collision

Simple picture: Evolution of displacement cascade



- **Defect accumulation and evolution:**
  - Reflection, sputtering
  - Initial kinetic energy

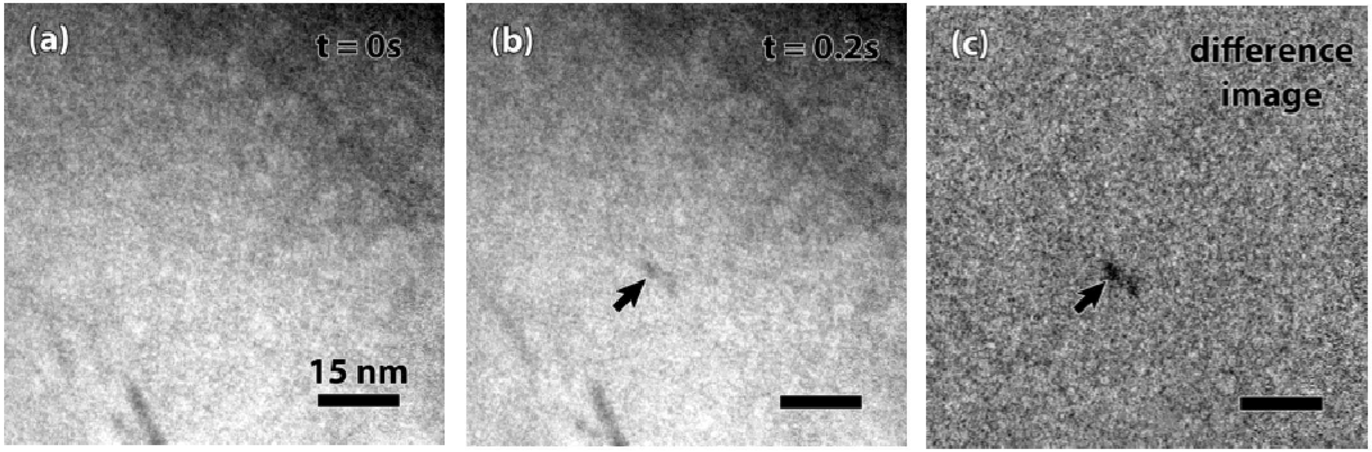
Simple picture: Long term damage



- **Long-term damage evolution:**
  - Primary damage production vs. diffusion and migration of defects
  - Damage recovery, sinks, defect trapping

Experimentally characterizing single ion strikes

- Experimentally identifying and characterizing complex isolated nanoscale damage events in materials is difficult:
  - Single ion/dopants implants, ion beam modification.



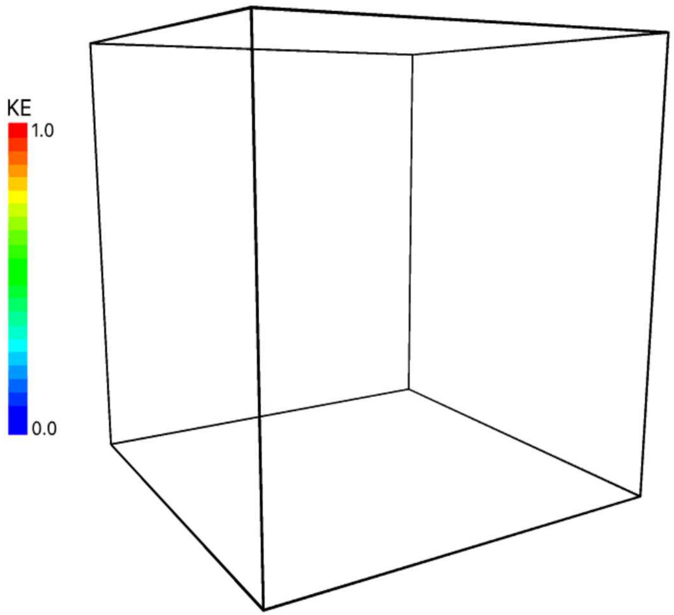
Individual frames taken from video collected in-situ in the TEM during irradiation of Si sample with 1.8 MeV Au^{3+}. Sample in a down-zone imaging condition near [123]-type zone axis. Single ion strike highlighted in difference image.

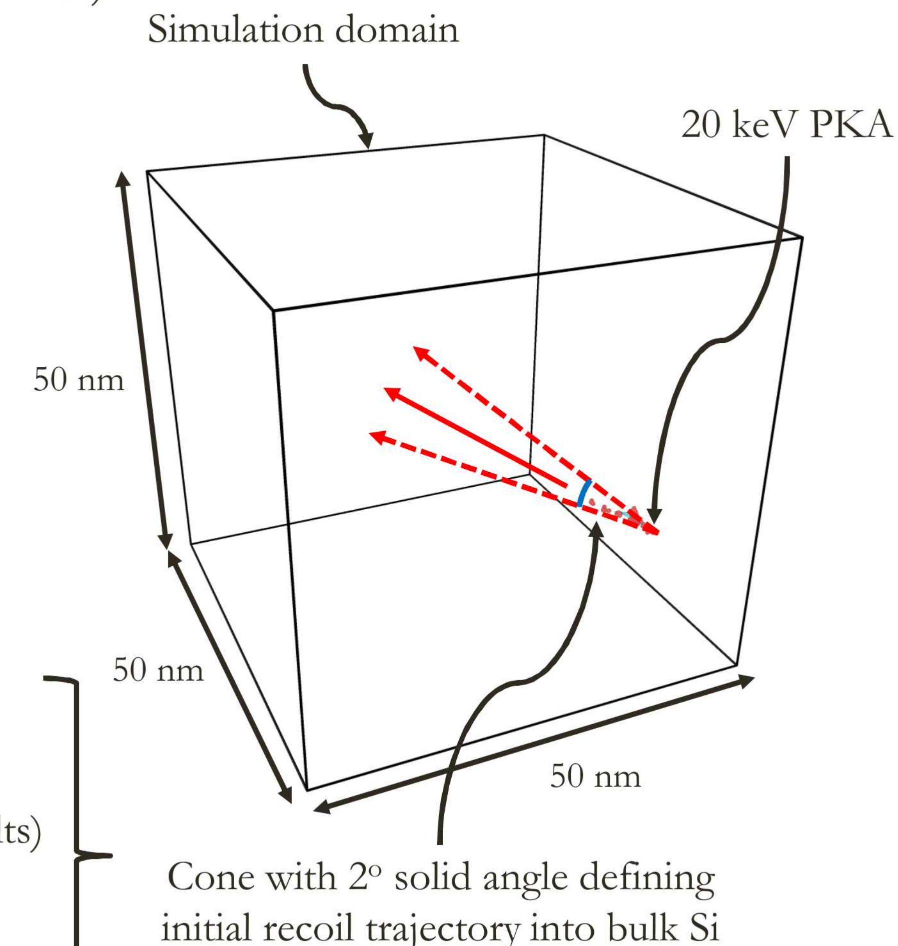
- Fundamental disconnect between simulation and experimental characterization tools – no information on defect structure or species.

- Virtual diffraction offers an opportunity to directly bridge atomistic simulations with experimental nanoscale characterization.

Simulating ion strikes with molecular dynamics

- LAMMPS atomistic code is used to perform simulations of multiple single PKA displacement cascades with a recoil energy of 20 keV into bulk Si (~46 keV Au).



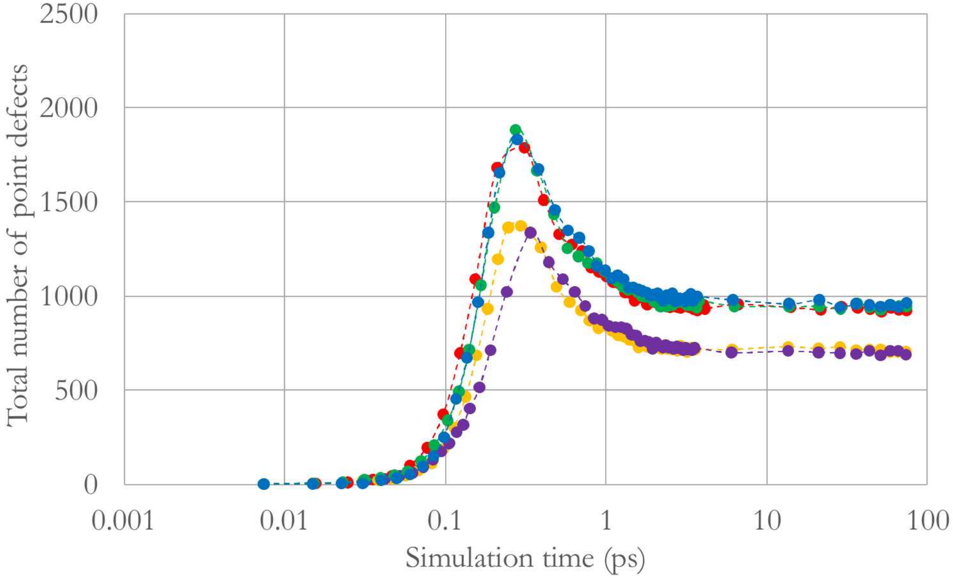


- Tersoff potential with:
  - ZBL nuclear repulsion correction
  - Electronic stopping effects (fit to SRIM results)

$$m_i \frac{\partial \mathbf{v}_i}{\partial t} = \mathbf{F}_i(t) - \gamma_s \mathbf{v}_i$$

- Boundary thermostat to absorb shockwave

Cascade damage analysis: Traditional approaches



Total number of point defects for all final defect structures

	Total number of final defects
Cascade 1	926
Cascade 2	704
Cascade 3	690
Cascade 4	946
Cascade 5	964
Average value	846
Standard deviation	137

- Maximum and final number of defects can vary greatly with only minor differences in PKA initiation
- Three simulations have maximum damage of ~1800 defects, other two have ~1350
  - Can it lead to greatly different diffraction signals?

- With Tersoff potential, $E_d \sim 16.9$ eV
- NRT model: $0.8E_{PKA}/2\,E_d = 473$ FPs (compared to 423 from these 5 simulations)

Cascade damage analysis: Traditional approaches

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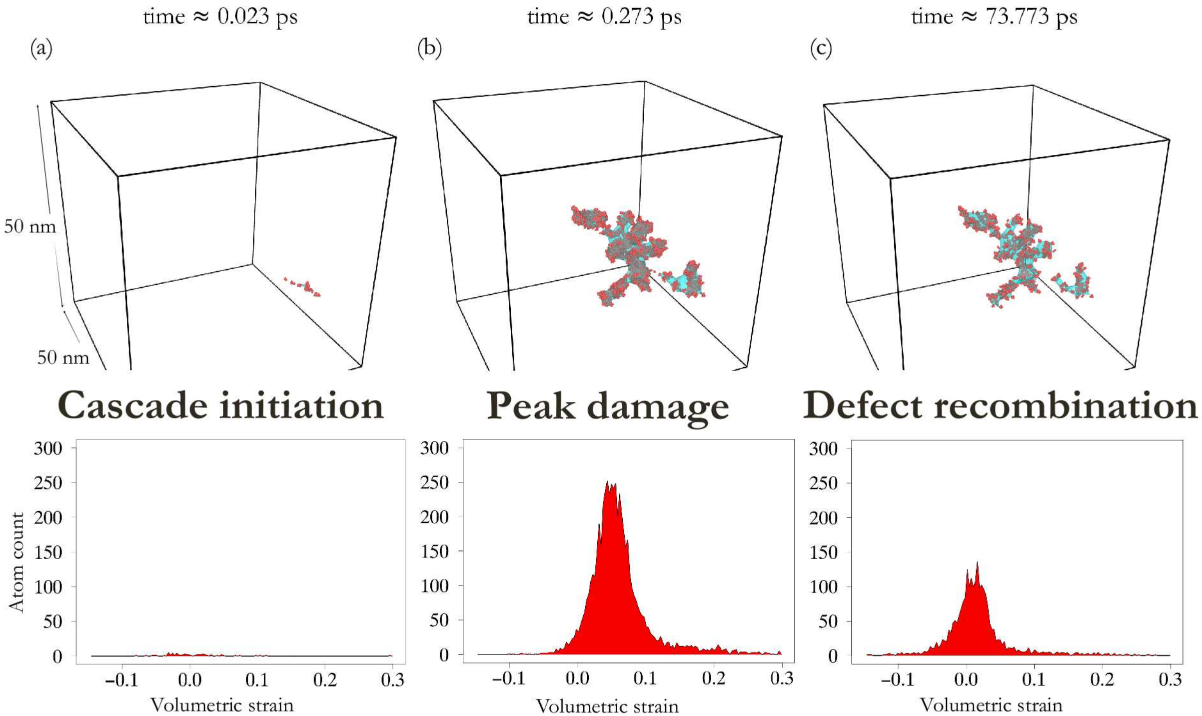


Average volumetric strain for all final defect structures

	Average strain	Standard deviation
Cascade 1	0.01368	0.03379
Cascade 2	0.01853	0.03457
Cascade 3	0.01439	0.03270
Cascade 4	0.01659	0.04628
Cascade 5	0.01538	0.03752

- Atomic strain has implications for atomic mobility and defect accumulation, can "appear" in SAED patterns
- Can it provide an indication as to the strength of the response expected in the SAED patterns for given initial conditions?
- All volumetric strain distributions and final average volumetric strains are positive (skewed right)
- Net positive volumetric strain consistent with formation volume of most stable FP
- Most atoms experiencing tensile eigen-strain

Virtual diffraction methodology

1. Create a **mesh of reciprocal space**. 3D rectilinear mesh with fine resolution without prior knowledge of the crystal structure.

2. Compute **diffraction intensities** at each point on the reciprocal space mesh using structure factor equations. Compute structure factor for all atoms within the simulation.

3. Analysis and visualization of diffraction intensities to produce **Selected Area Electron Diffraction (SAED) and X-Ray Diffraction (XRD) patterns**.

All atoms are sampled at each reciprocal point within $\boldsymbol{K}_{\mathrm{max}}$ to determine the diffraction intensity, I:

$$I\left(\mathbf{K}\right) = L_p F\left(\mathbf{K}\right) F^*\left(\mathbf{K}\right)$$

$$F\left(\mathbf{K}\right) = \sum_{j=1}^{N} f_j \exp\left(2\pi \mathbf{i} \mathbf{K} \cdot \mathbf{r}_j\right)$$

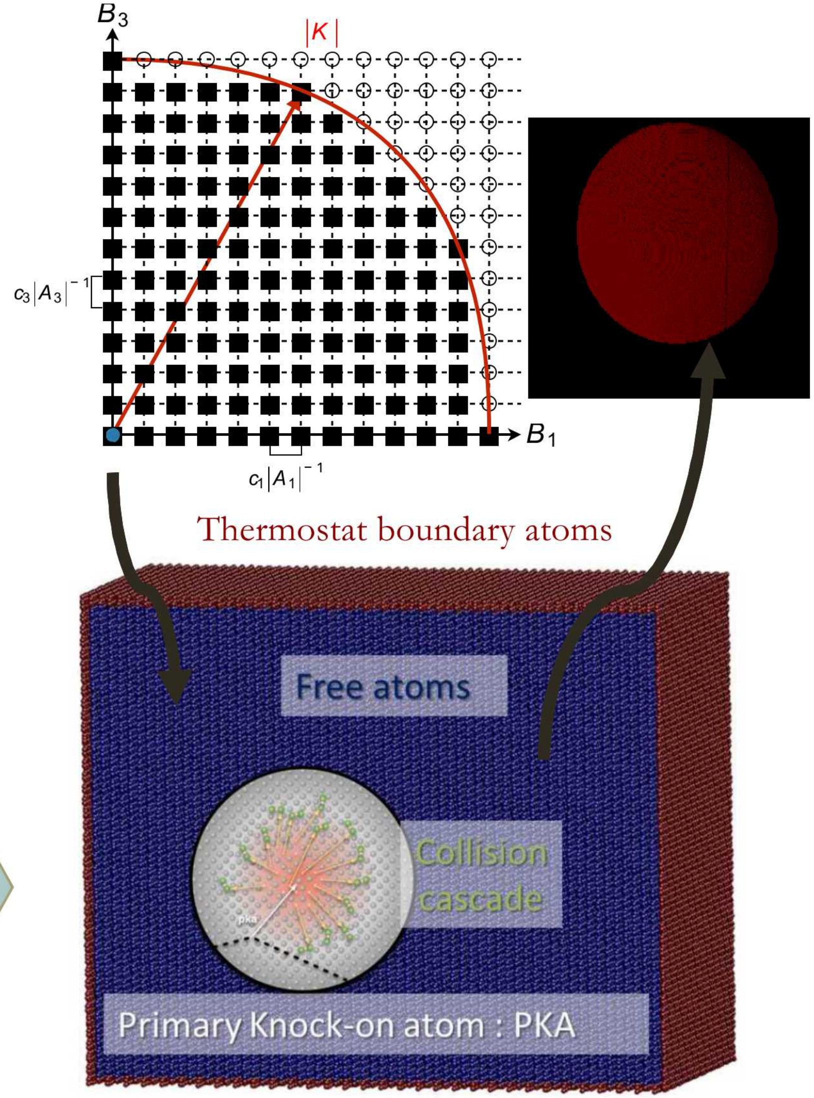
F = Structure factor

$\mathbf{K}$ = Reciprocal lattice point

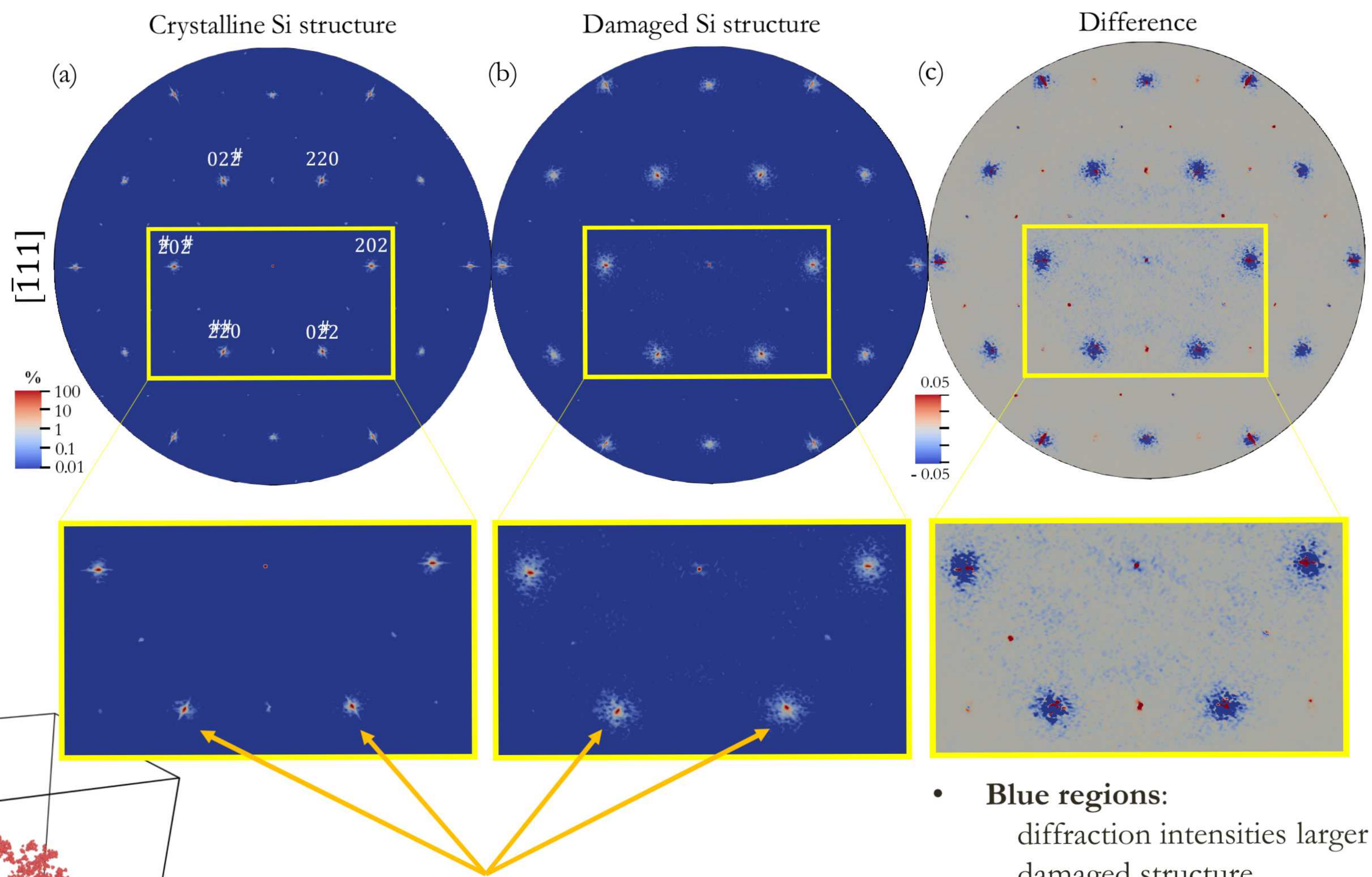
N = Number of atoms

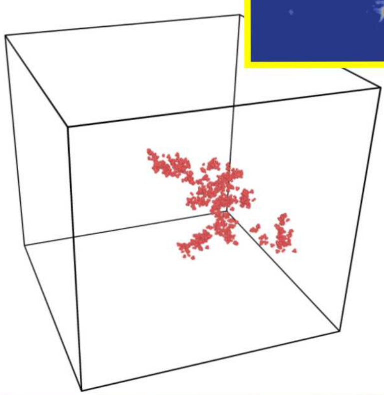
f_j = Atomic scattering factor

$\mathbf{r}_j$ = Atom position



Virtual diffraction of simulated cascade damage



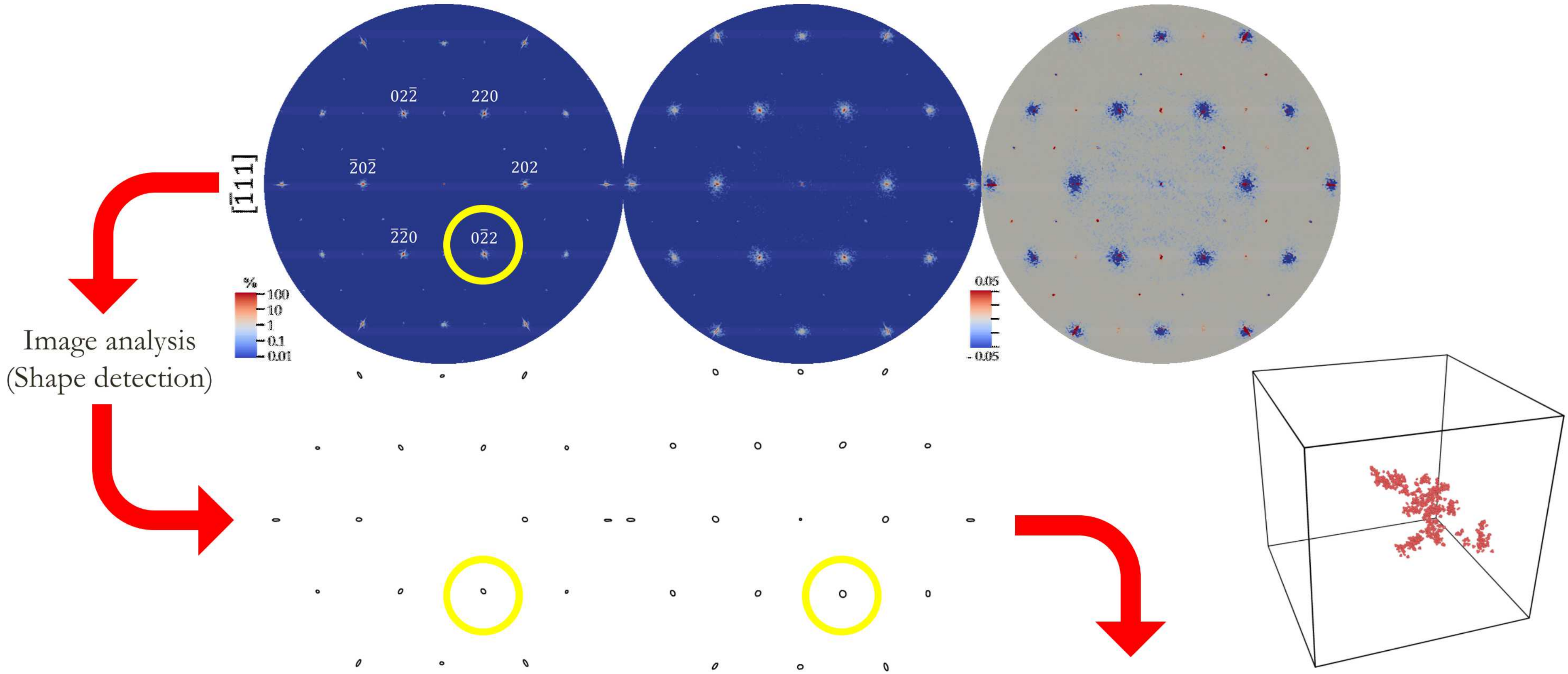


Spots have broadened…

200 keV e⁻ (λ = 0.0251 Å)

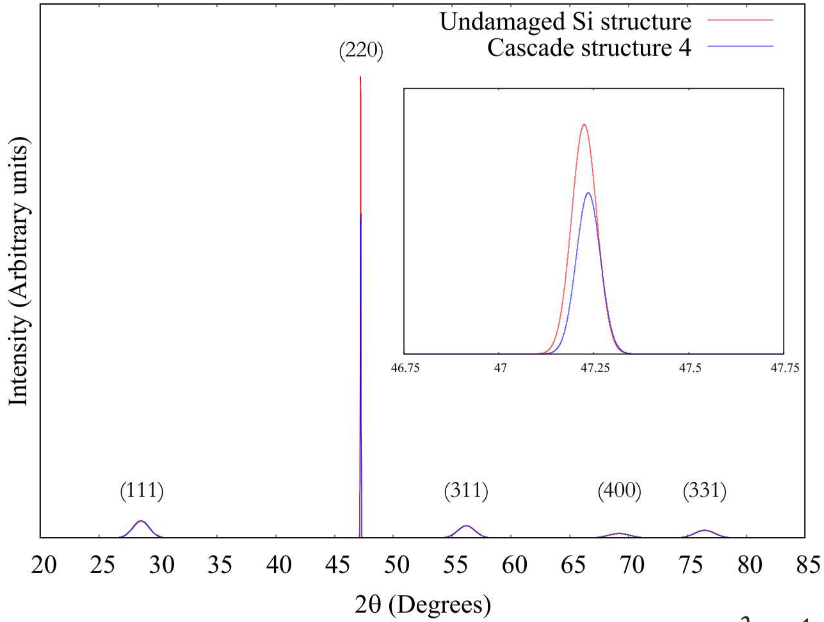
- **Blue regions**:
  diffraction intensities larger in damaged structure
- **Red regions**:
  diffraction intensities larger in undamaged structure

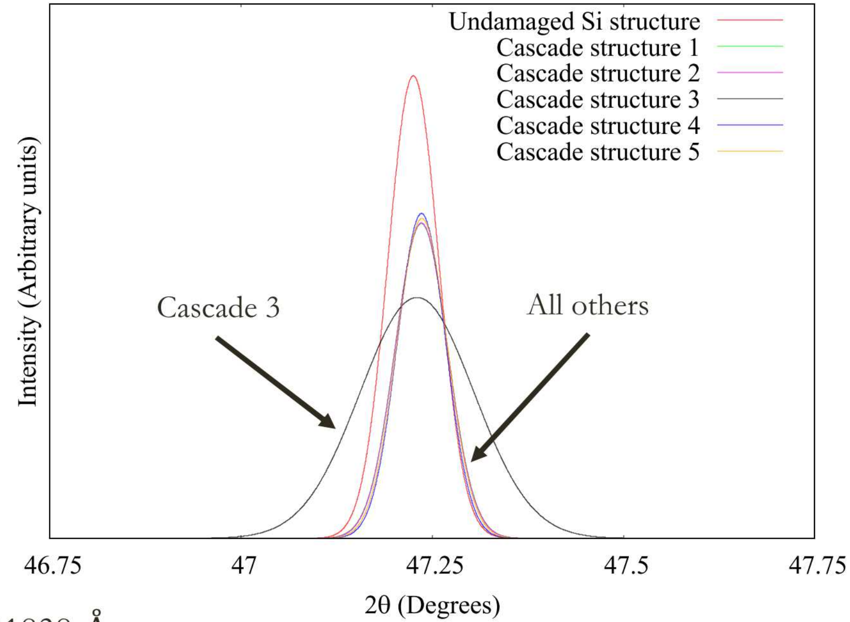
Virtual diffraction of simulated cascade damage



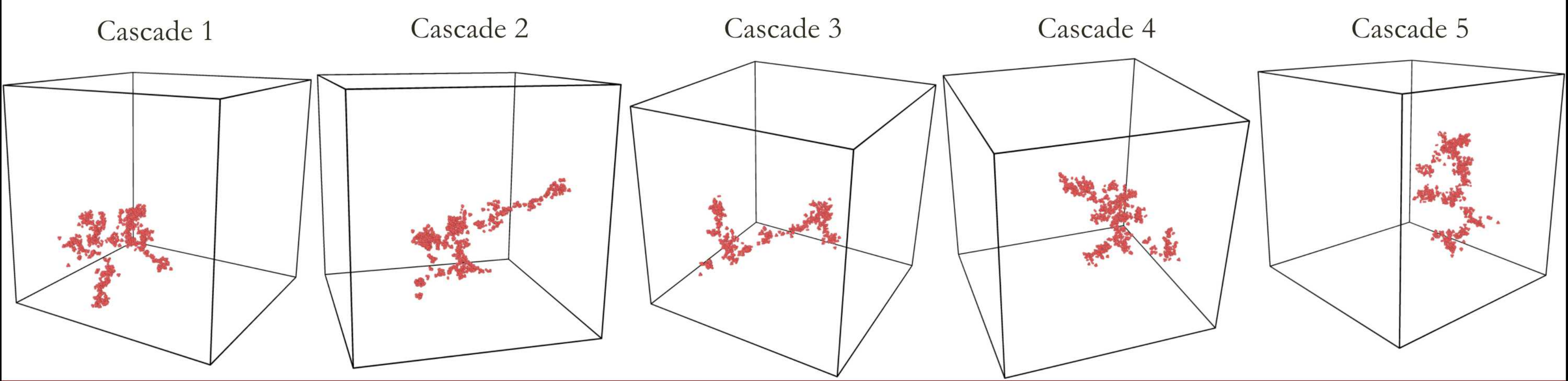
Spot: $0\bar{2}2$	**Perfect**	**Damaged**	**Change**
Radial distance (A^{-1})	0.5198889	0.5239566	0.0040677
Area (A^{-2})	0.0004956	0.0008242	0.0003286
Angle (degrees)	60.03	60.05	0.02
Ellipticity (A^{-1}, A^{-1}, degrees)	(0.03000613, 0.02102889, 128.02)	(0.03772318, 0.02781725, 135.22)	(0.00771705, 0.00678836, 7.2)

Virtual diffraction of simulated cascade damage

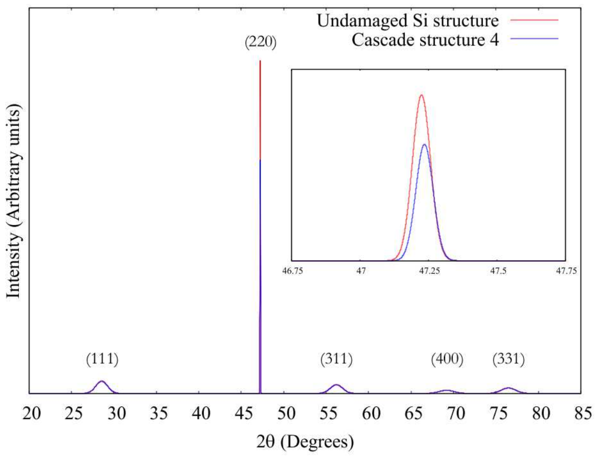


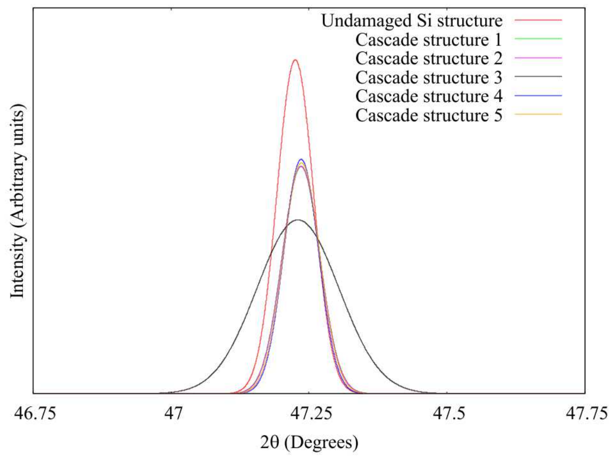


$\lambda = 1.541838$ Å



Virtual diffraction of simulated cascade damage





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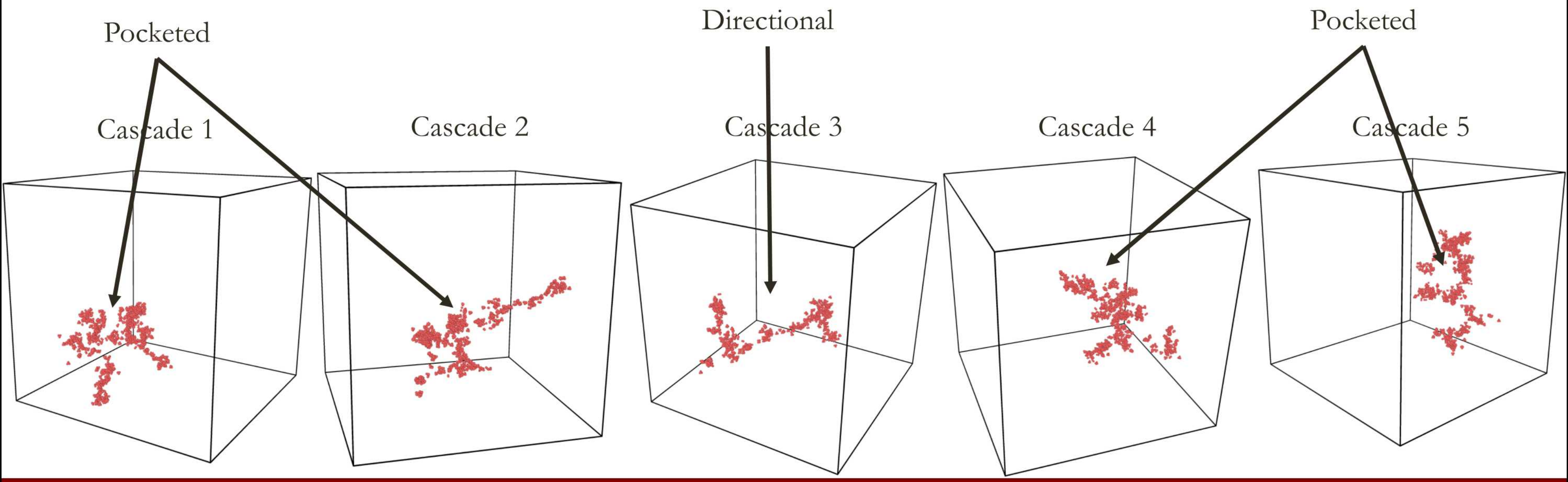
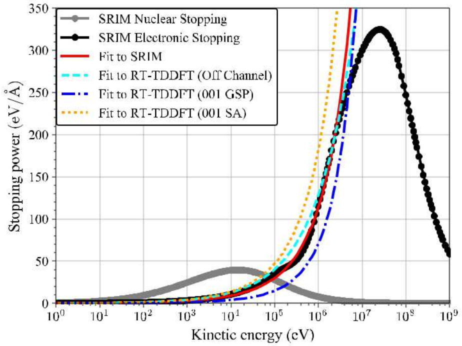
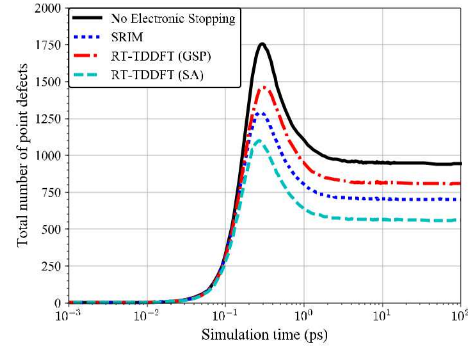
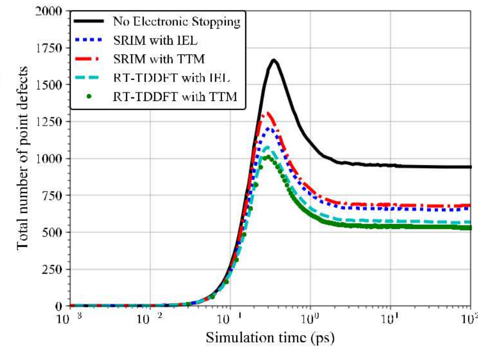


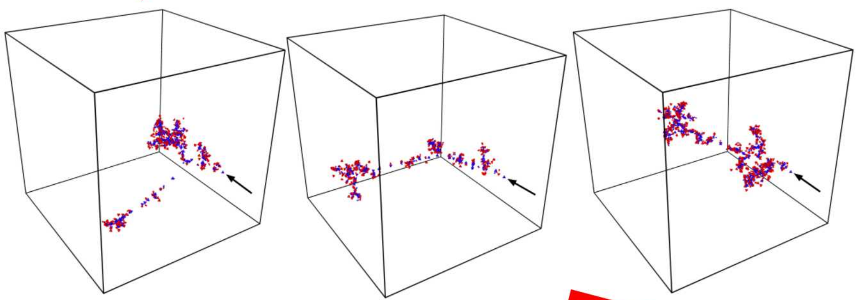
Summary: Atomistic modeling of ion strikes

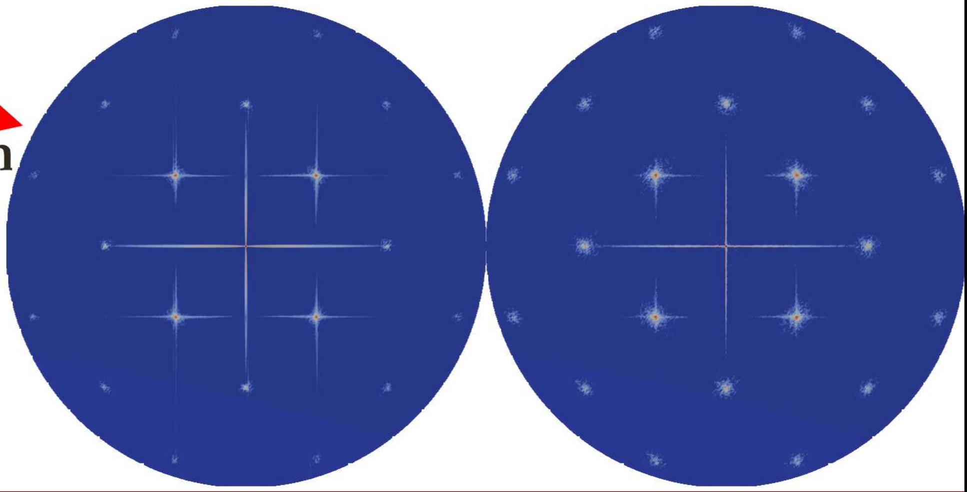


Use **atomistic methods to characterize ion strikes** from electronic structure through experimental signal









Assist experimental characterization efforts through virtual diffraction

- Can we eventually extract structural information from the diffraction signal?

Example 2: Shock Behavior

Gaining Insights on the Role of Crystal Structure on Shock Hugoniot Relations for HNAB via MD

Current experiments and related needs

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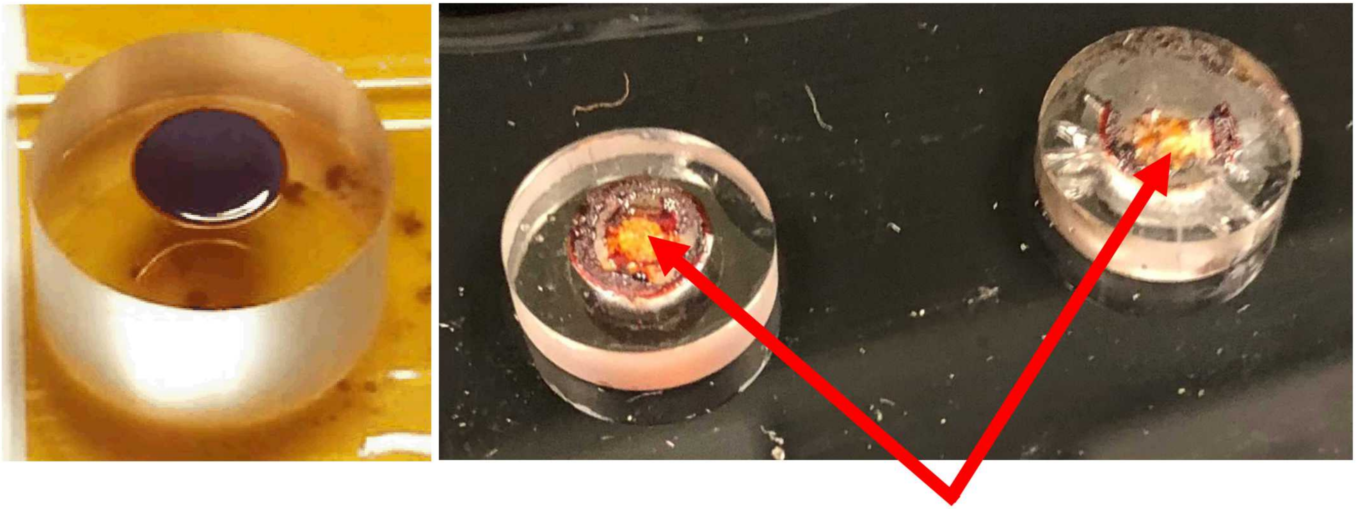
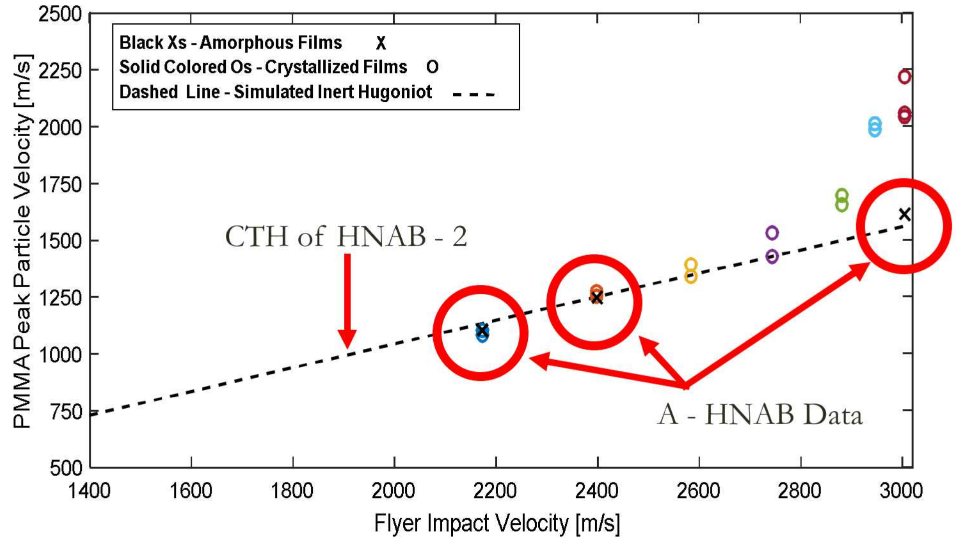
A - HNAB

Shocked A - HNAB (via flyer plate)

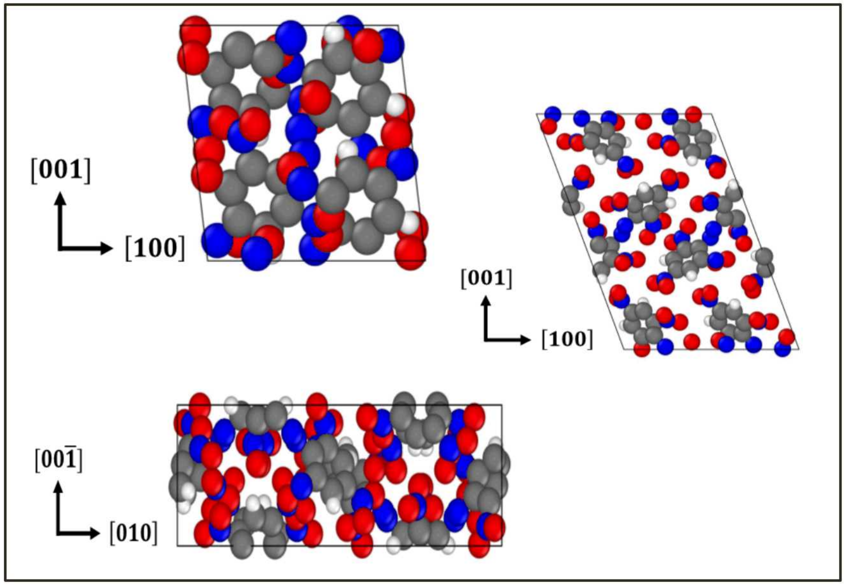


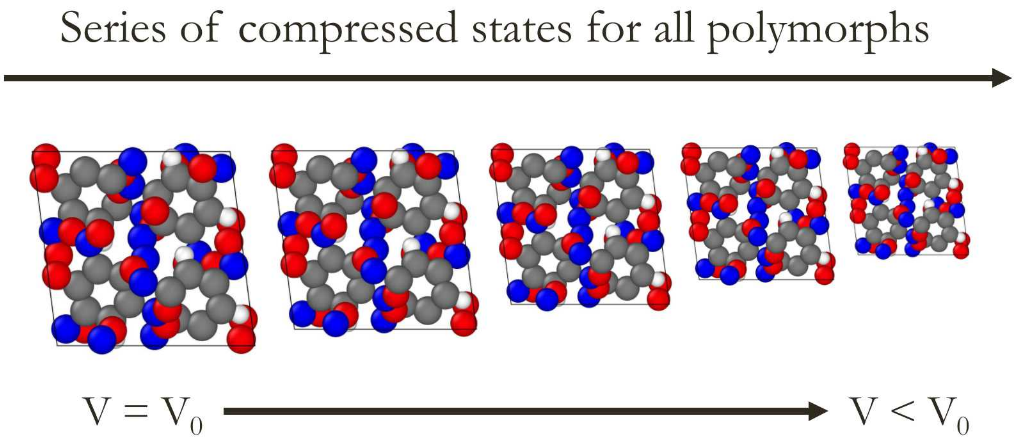
Shock induced crystallization (mixture of structures?)

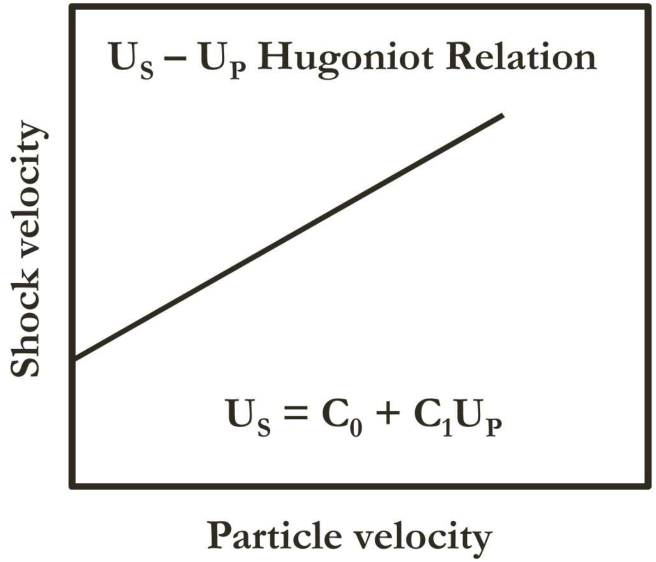


- The Hugoniot describes the relationship between the material **states on both sides of a shock wave.**
- A **calculated inert Hugoniot can provide guidance** as to where the experimental particle velocities should be for various flyer impact velocities.

Finding the Hugoniot state (P, T, E) for any V







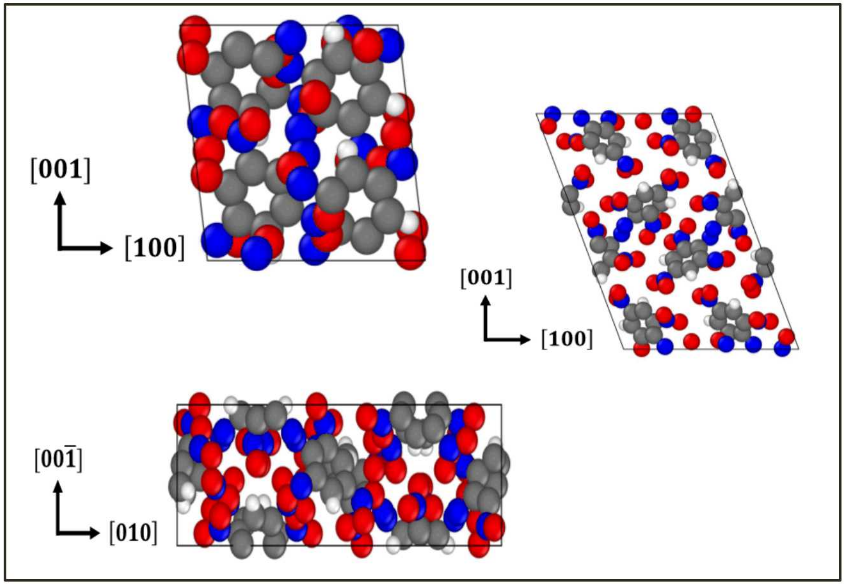
Mass Conservation: $\rho_0 D = \rho_1 (D - u_1)$

Momentum Conservation: $P_1 = \rho_0 D u_1$

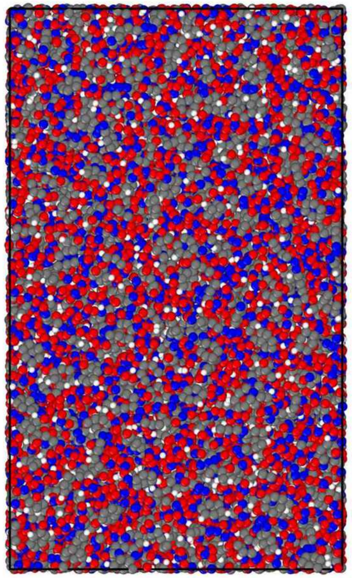
Energy Conservation: $E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$

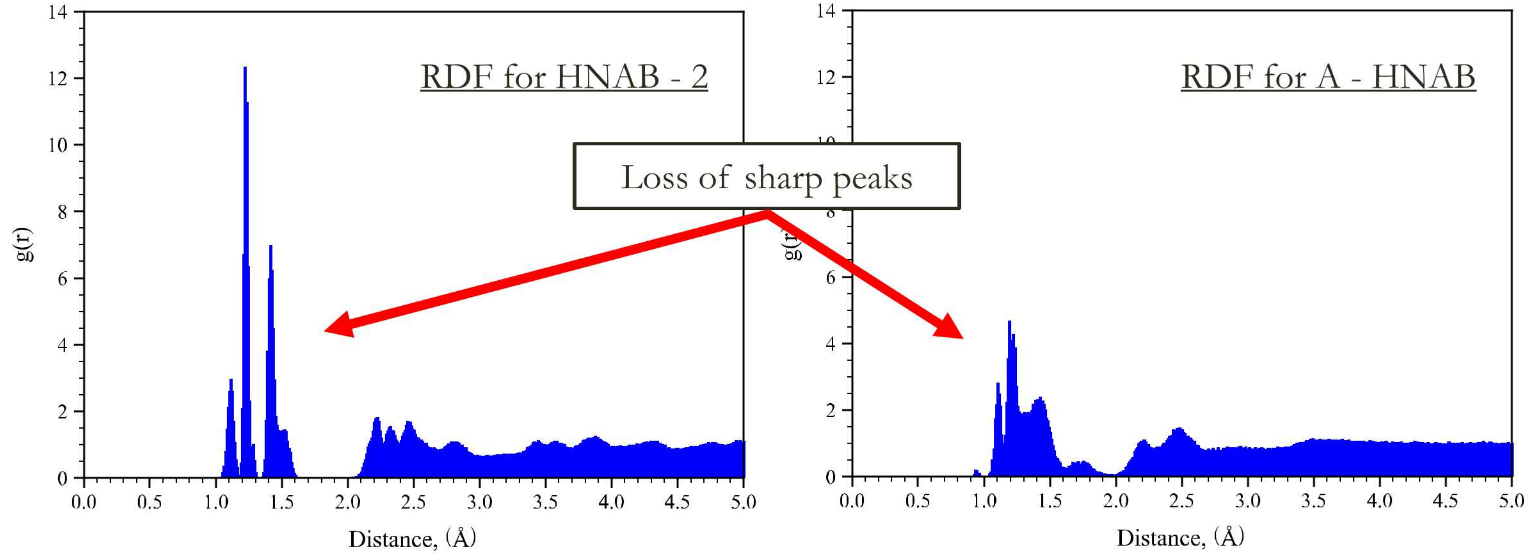
Approach: Set $V < V_0$, ~ 300 K equilibration, ramp T, solve for T where Rankine-Hugoniot condition is true.

MD reference structures for HNAB



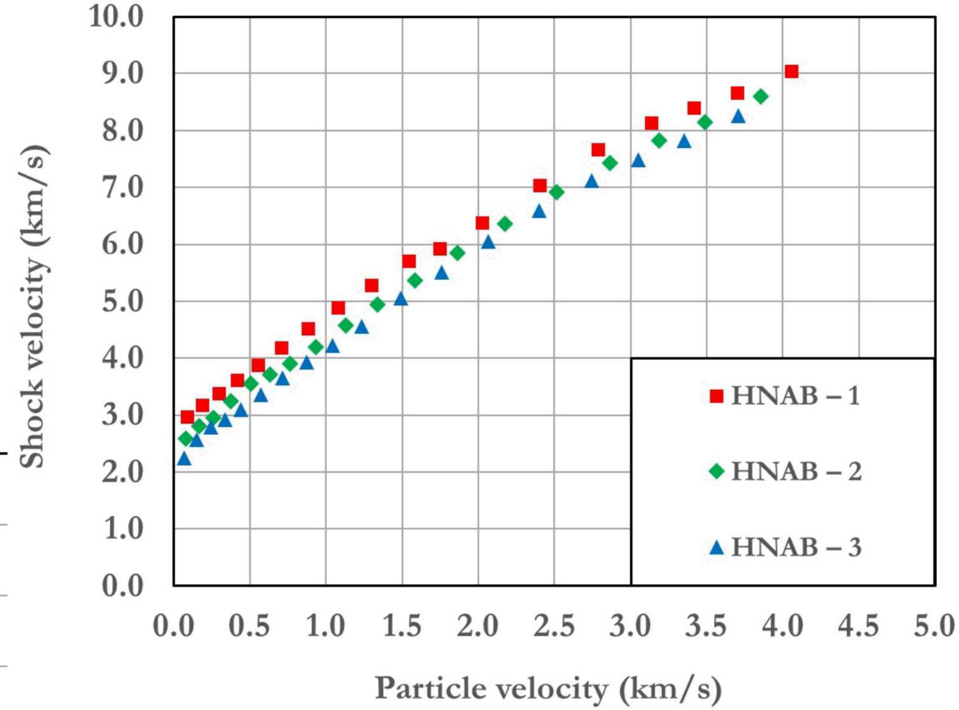
Melt the structure!

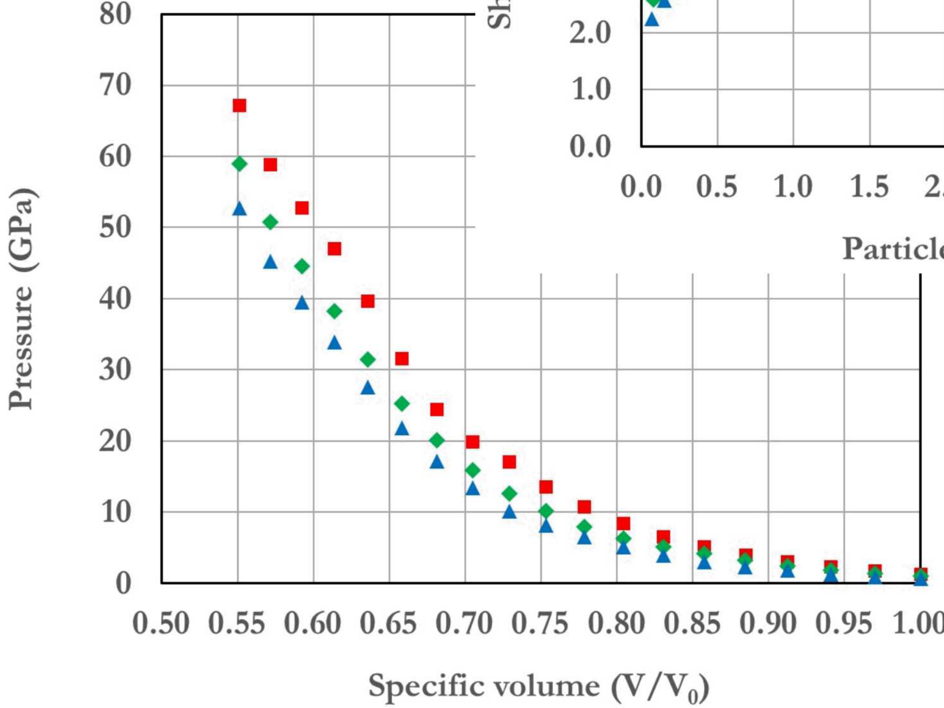




Calculated crystalline HNAB Hugoniot

Experimental point-of-view

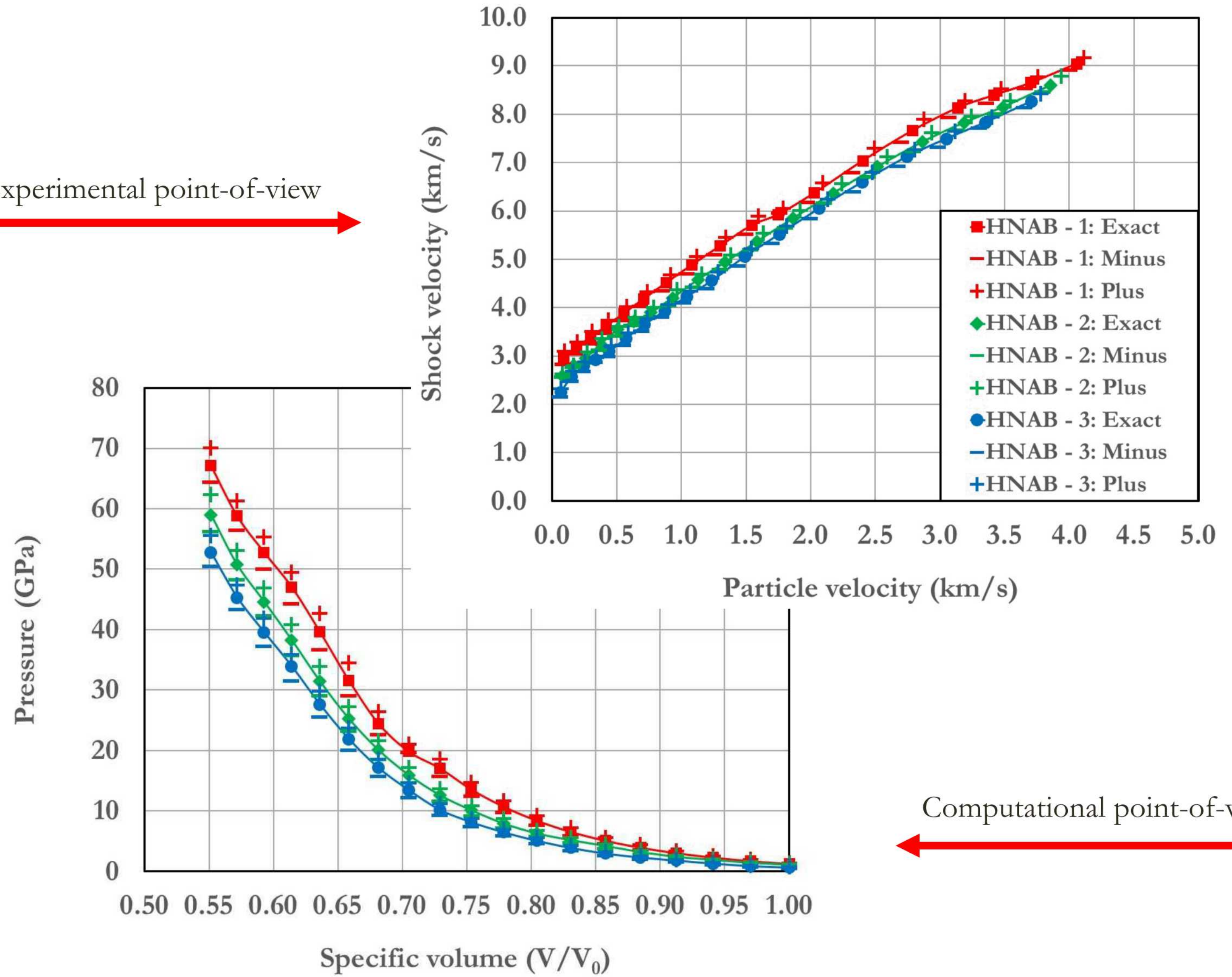




Computational point-of-view

Effect of density variations in HNAB Hugoniot

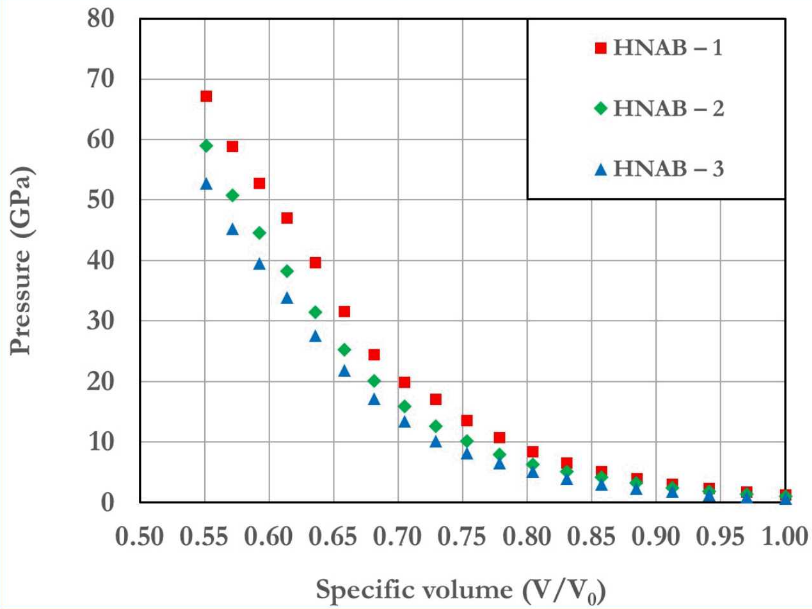
Experimental point-of-view

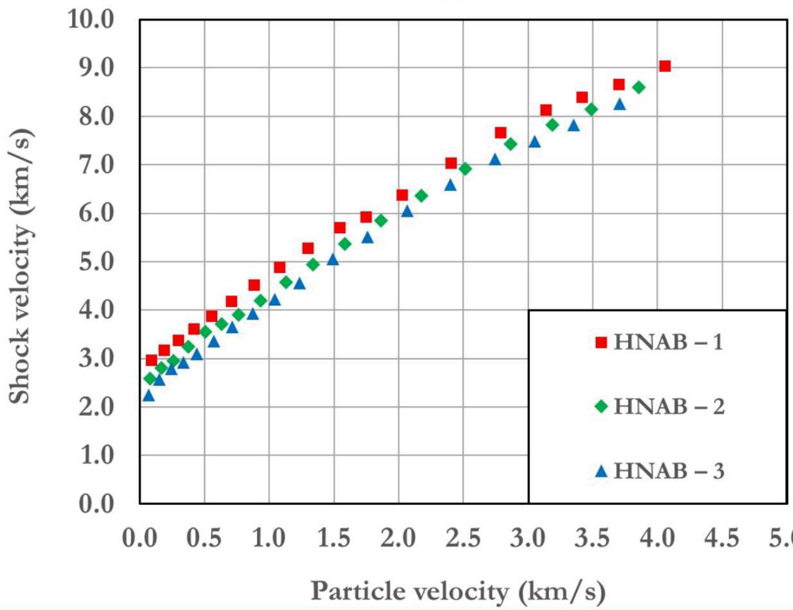


Computational point-of-view

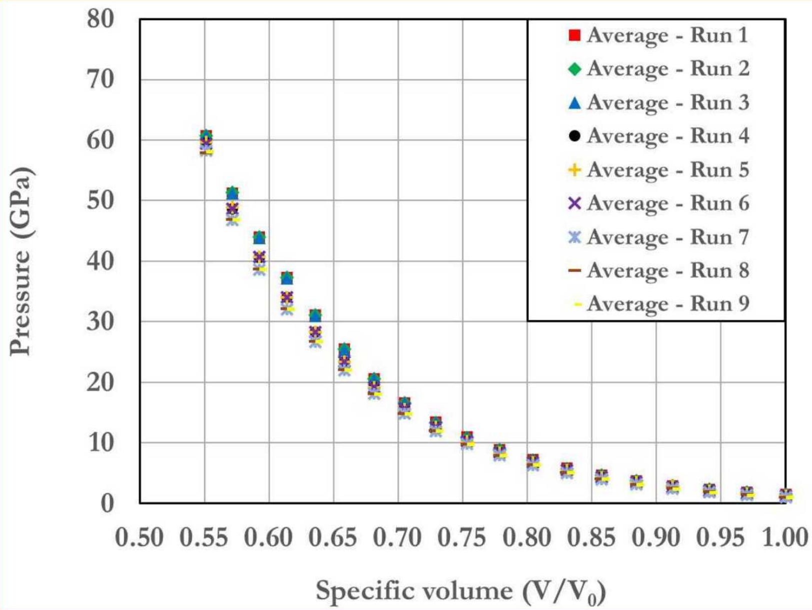
Calculated crystalline vs. amorphous Hugoniot

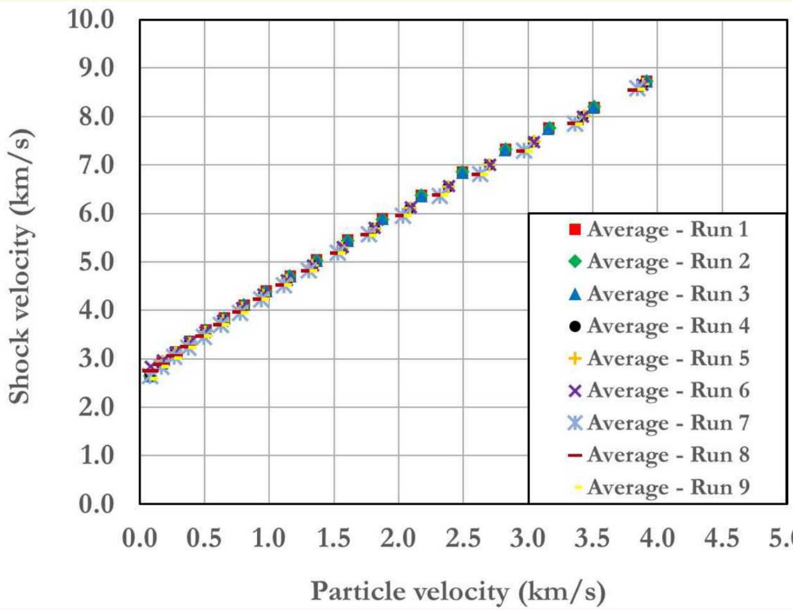
Crystalline





Amorphous



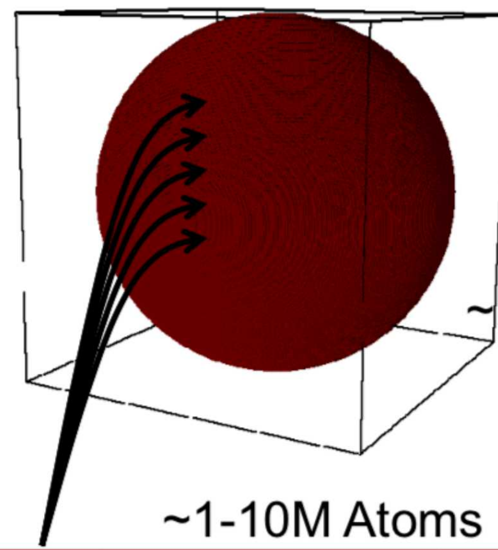


Virtual diffraction methodology

Diffraction intensity is calculated at each reciprocal lattice node using the structure factor: diffraction conditions satisfied with nodes located on Ewald sphere surface.

$$I(\mathbf{K}) = \mathrm{Lp}\, F(\mathbf{K}) F^*(\mathbf{K})$$

Lp = Lorentz-Polarization Factor (only XRD)
F = Structure Facture
$\mathbf{K}$ = Reciprocal Lattice Point (Relp)



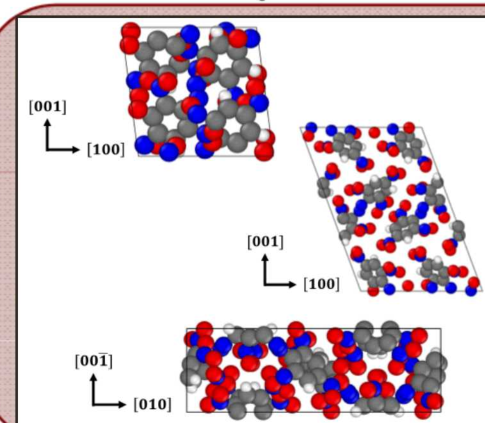
~10-100M Relp

Structure Factor:

$$F(\mathbf{K}) = \sum_{j=1}^{N} f_j \exp\left(2\pi i\, \mathbf{K} \cdot \mathbf{r}_j\right)$$

N = Number of Atoms in Simulation
f_j = Atomic Scattering Factor
$\mathbf{r}_j$ = Atom Position

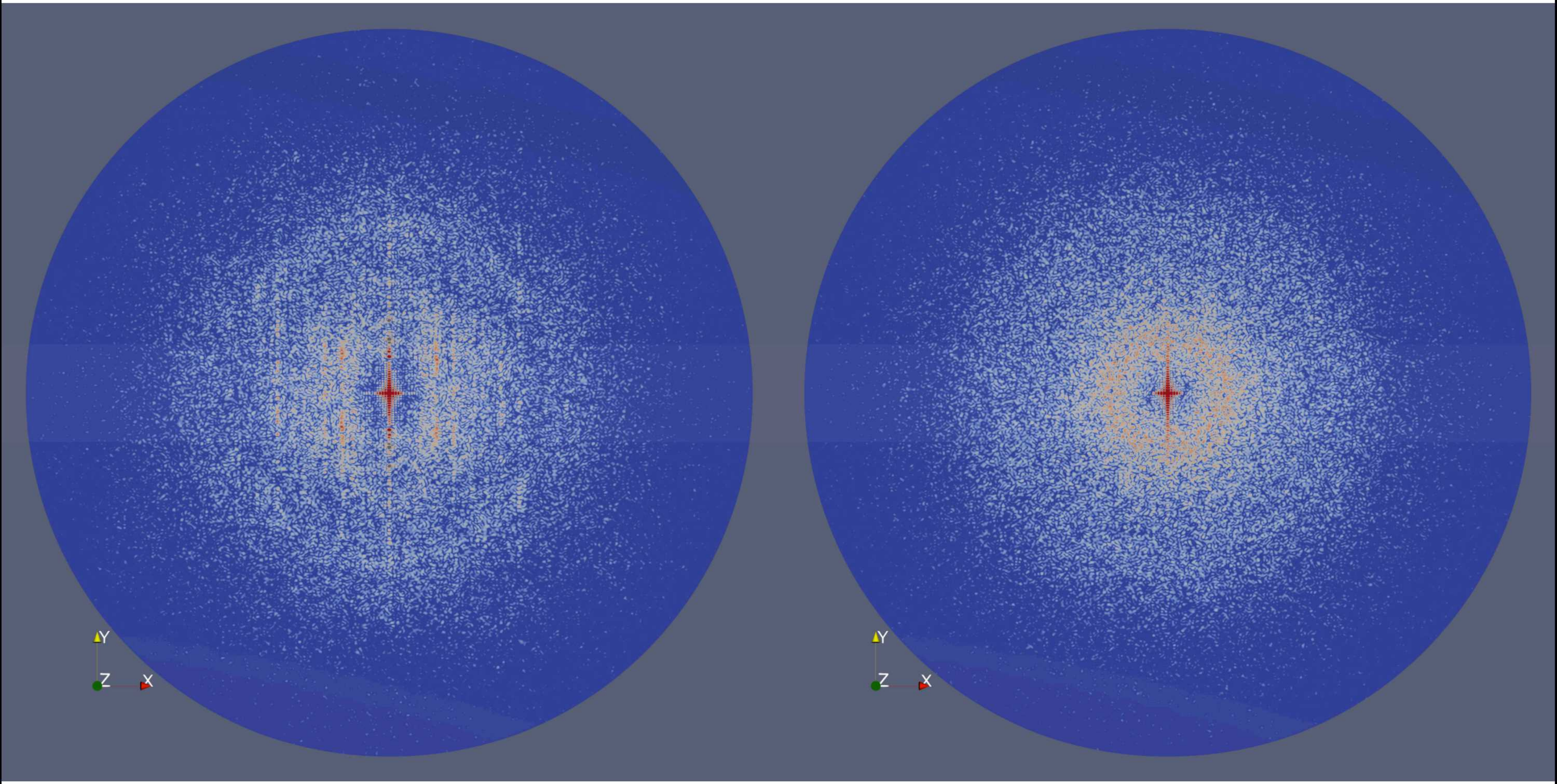
~1-10M Atoms



All atoms are sampled at each reciprocal point.

SAED of compressed HNAB microstructures

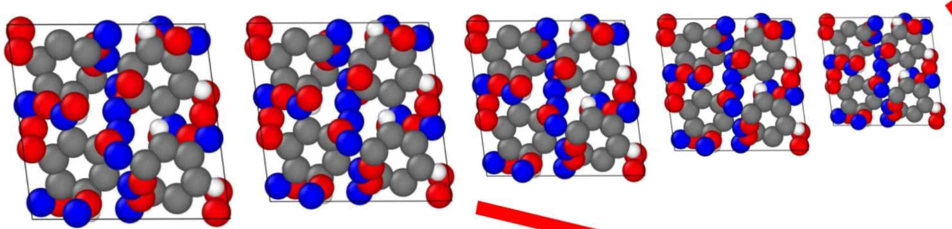
HNAB - 2 | A - HNAB

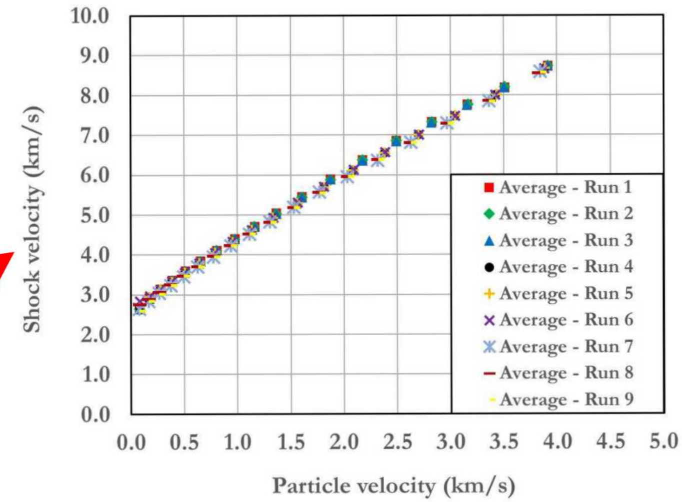


Summary: Atomistic modeling insights of Hugoniot

Using **atomistic tools to characterize shock behavior** in a high-throughput way (~10k sims)

- General method for full EOS characterization
- Provides input and sensitivity analysis for CTH calculations and guides experimental data analysis





Assist experimental characterization efforts through virtual diffraction

- Determination of phases present
- Phase transformation during compression