Building a Virtual Framework to Model Laser Shock Experiments

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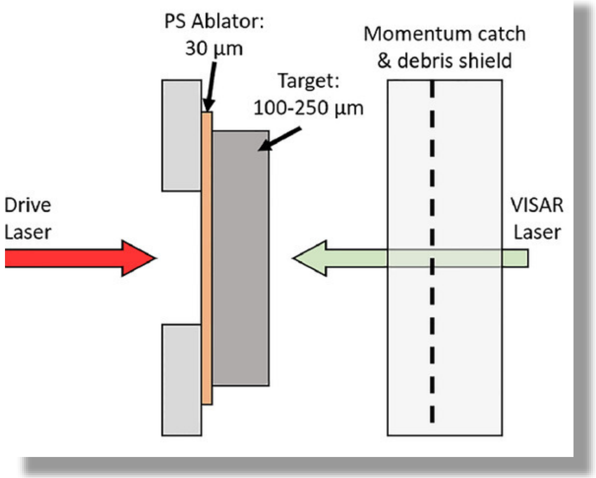
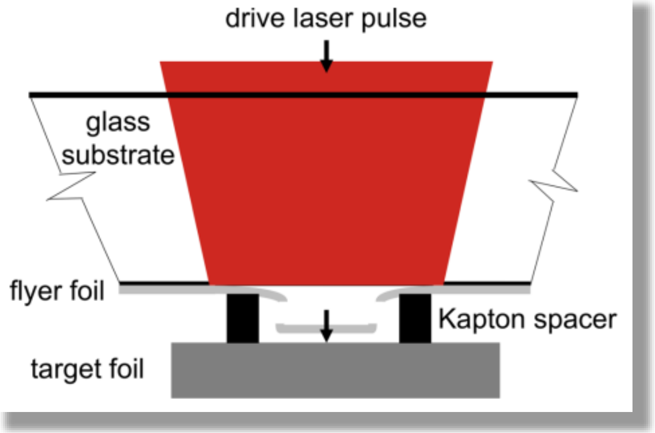
2023 HEDS Seminar Series

26th Jan 2023

Laser Shock Experiments

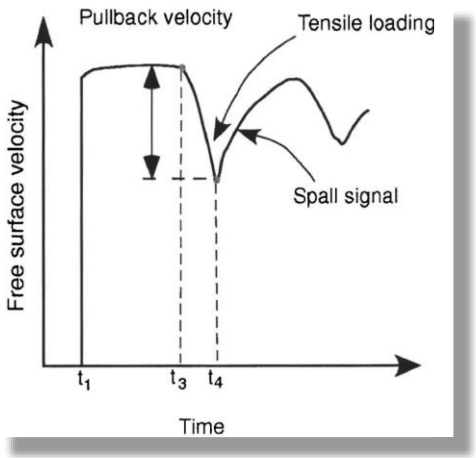


[Righi et al., Acta Mater (2021)]

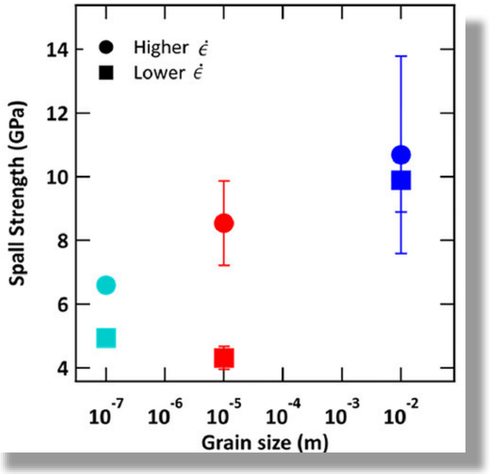


[D. D. Mallick et al. *Exp. Mech.* (2019)]

Rear surface velocity



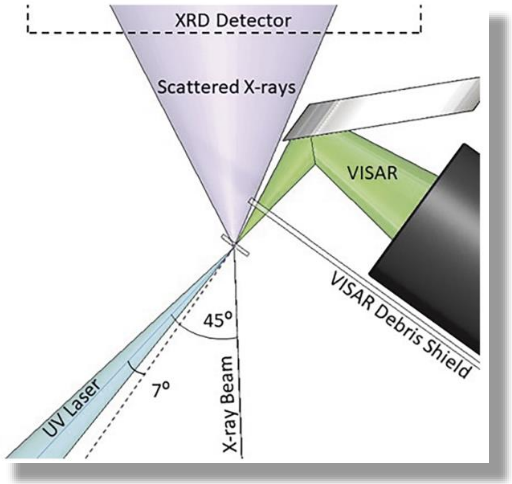
[Chen, et al., JAP (2006)]



[Righi et al., Acta Mater (2021)]

- *Rear surface velocity:* spall strength, strain rate, Hugoniot elastic limit, phase transformation behavior
- Strain Rates > 10^7 s^{-1}. ; Small samples (< few hundred microns)
- **Challenge:** Predicting the plasticity contributions in BCC metal microstructures

In situ Characterization of Dynamic Deformation Behavior of BCC Metals

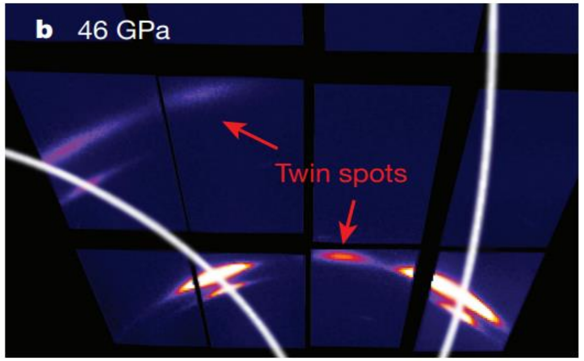


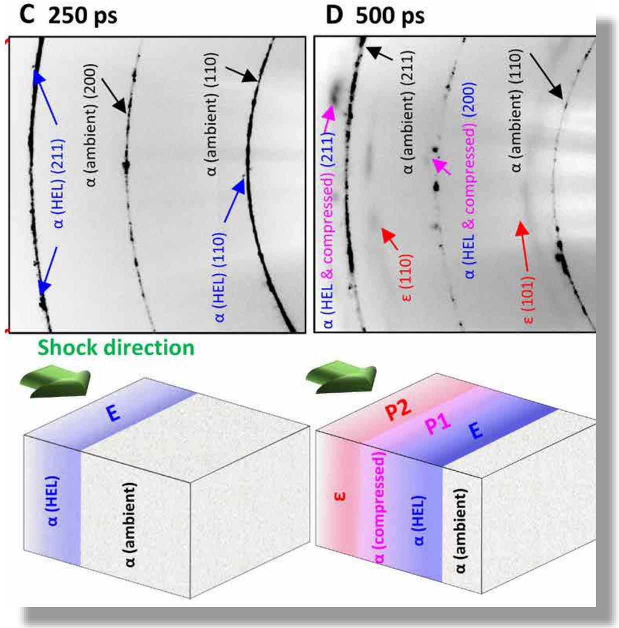
[Wang et al., Rev. Sci. Instrum. (2019)]

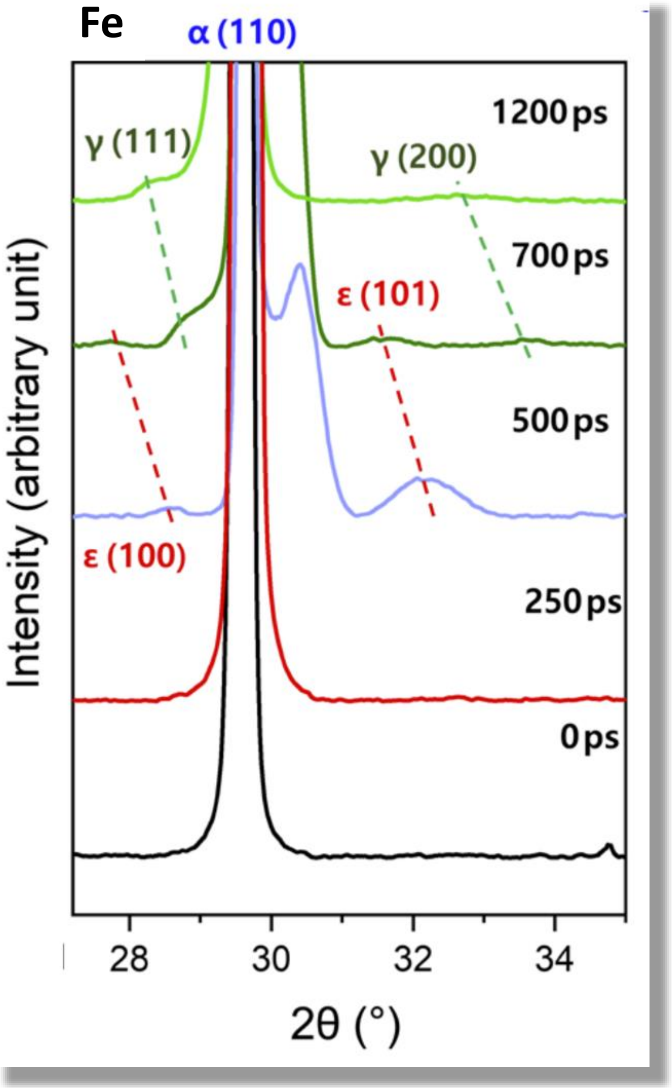
- Peak broadening (defects)
- Peak splitting (twins) or
- New peaks (phase transformation)

Quantification of fractions of twins or phase fractions and dislocation density.

Ta [Wehrenberg et al., *Nature* (2017)]





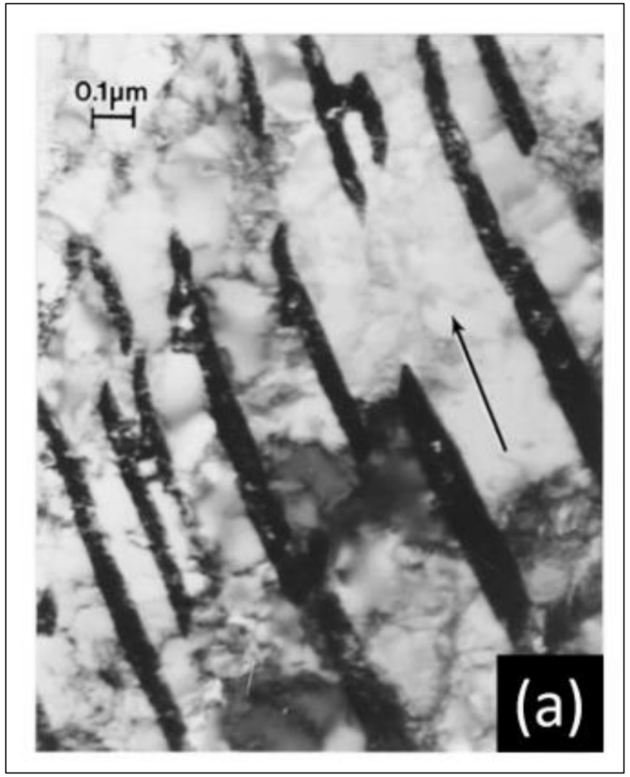


[Hwang et al., *Sci. Adv.* (2020)]

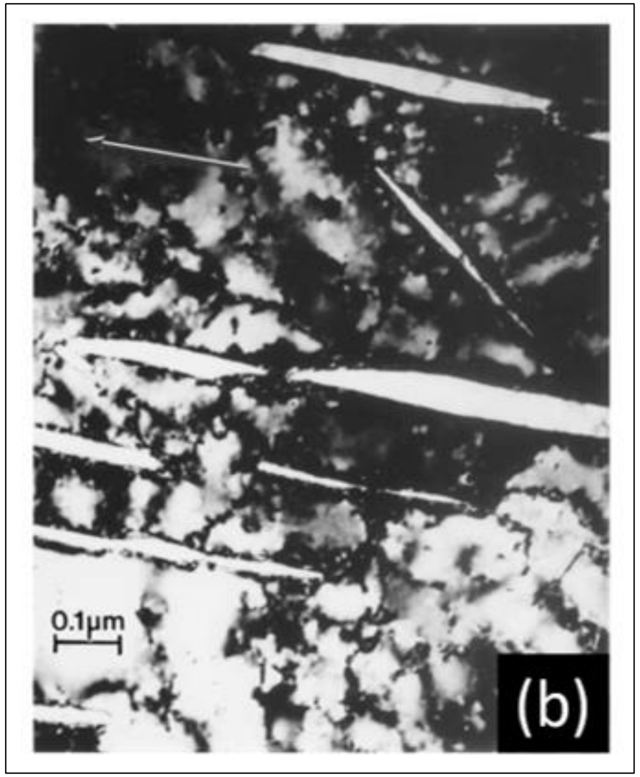
Shock Recovery Experiments: Plasticity Contributions

[Murr and Esquivel, J. Mater. Sci. (2004)]

[Want et al., Sci. Rep. (2013)]



Ta



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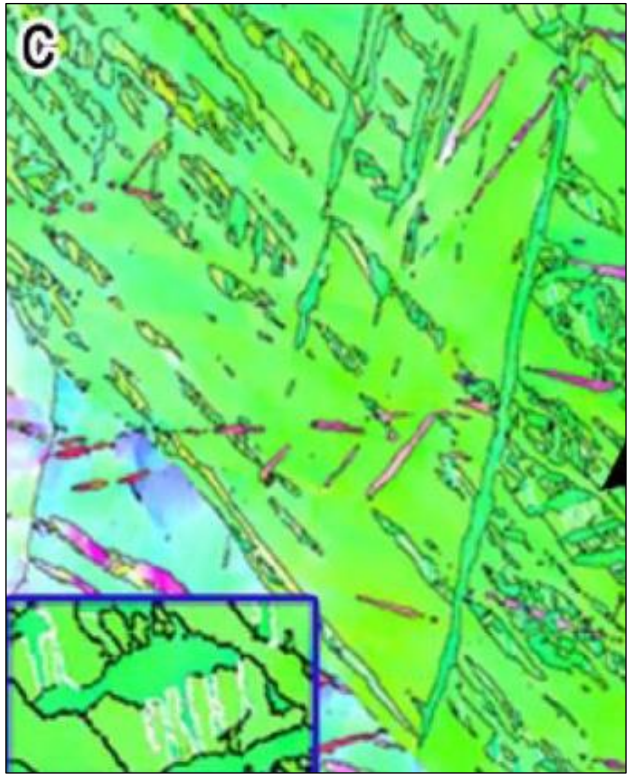
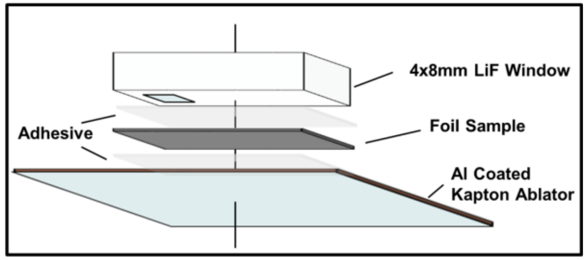


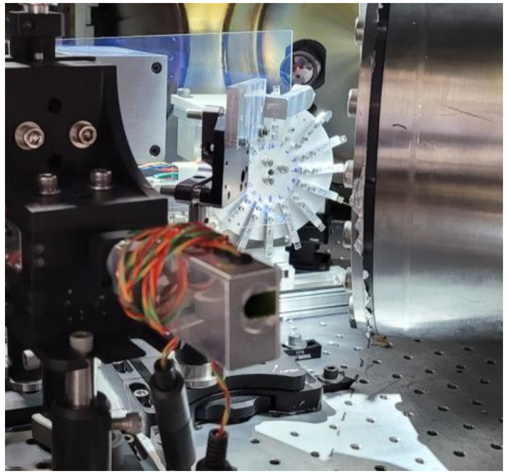
Fe

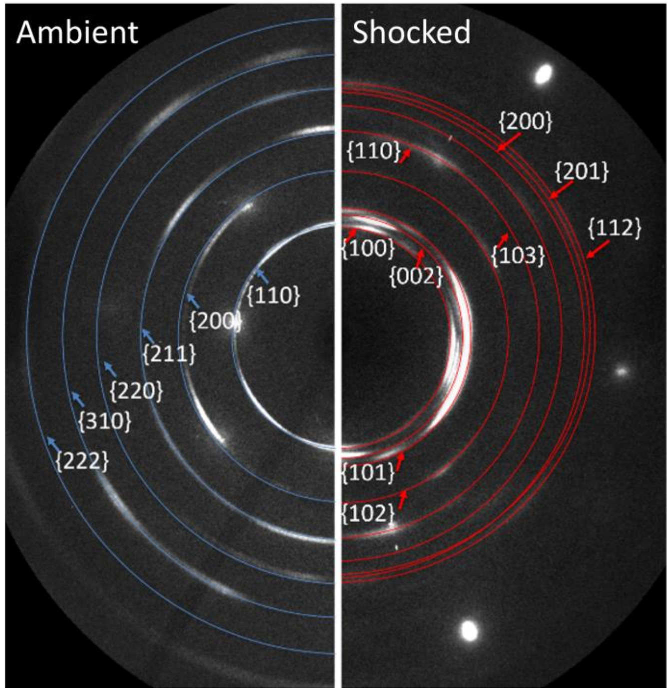
- **BCC Metals: Dislocation twins and dislocation density in Shock-recovered BCC metals**
  - Correlations between shock stress or strain rate and twinnability → critical twinning stress

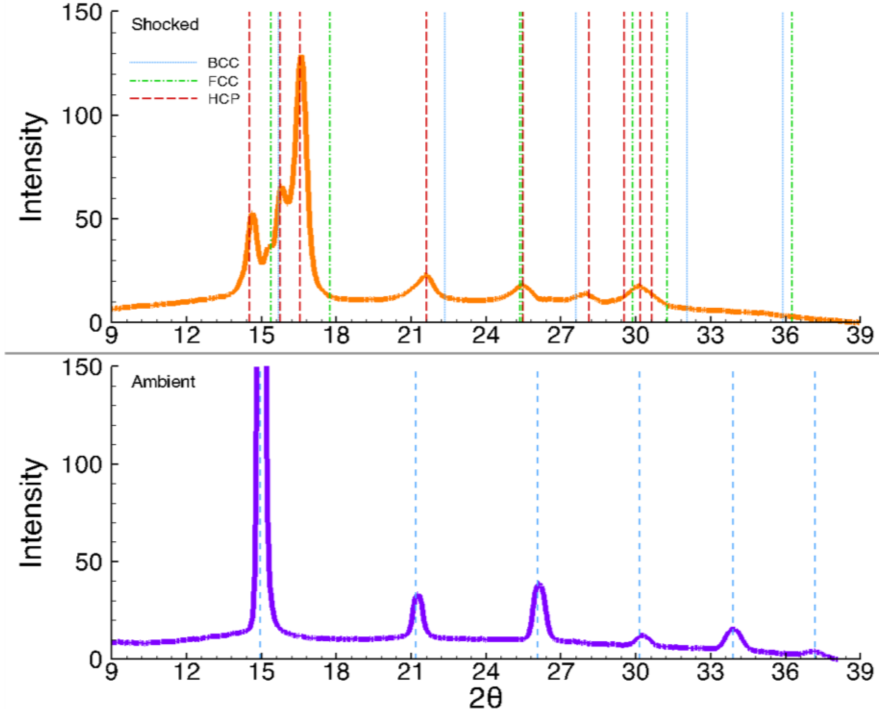
In Situ Diffraction Experiments at DCS

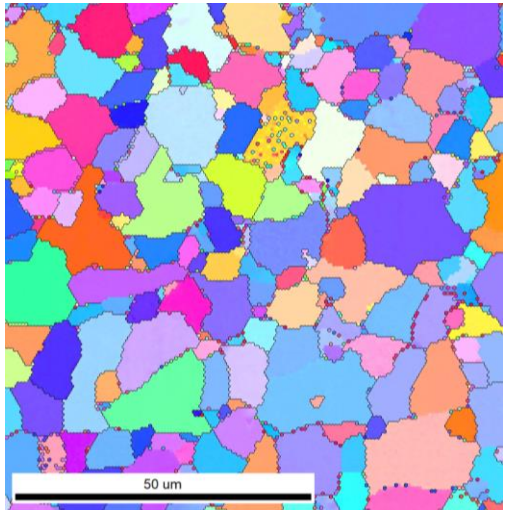
- 100J laser system (10 ns pulse)
- ~25 µm thick Fe foils





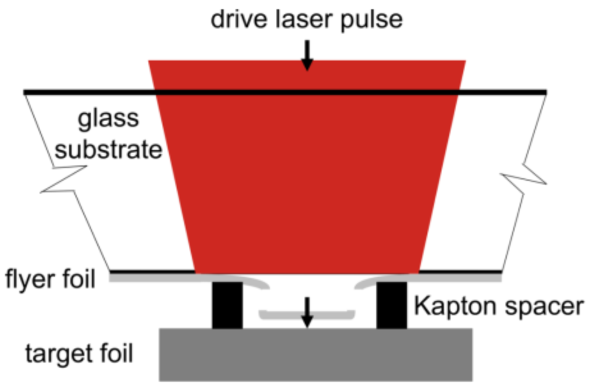




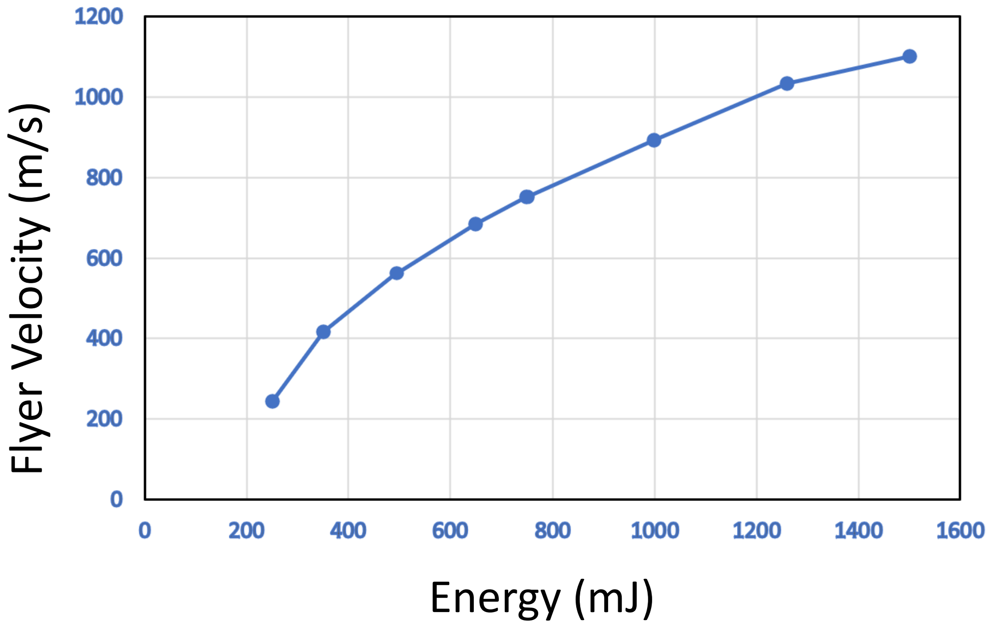


Interpretation of diffraction patterns is difficult if mixed stress states (partial compressed/release)

Laser-Driven Micro-Flyers

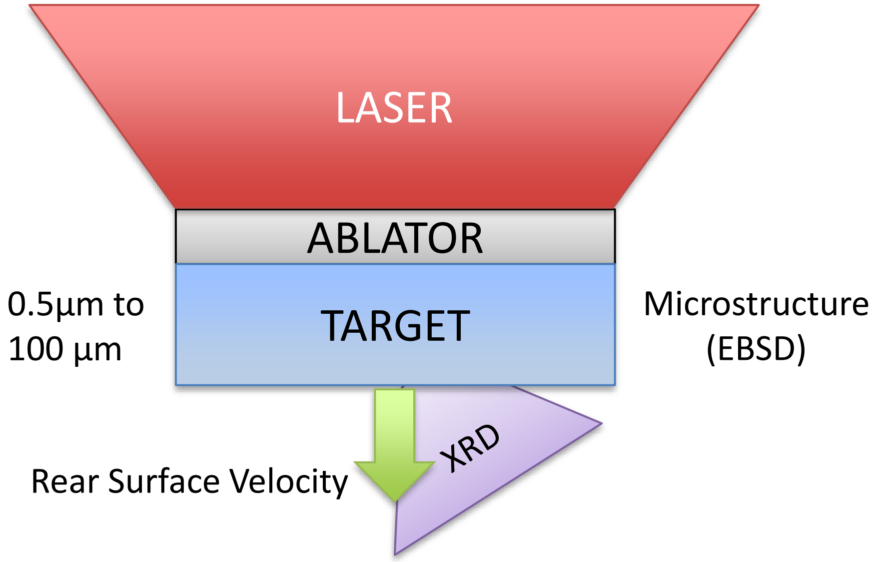


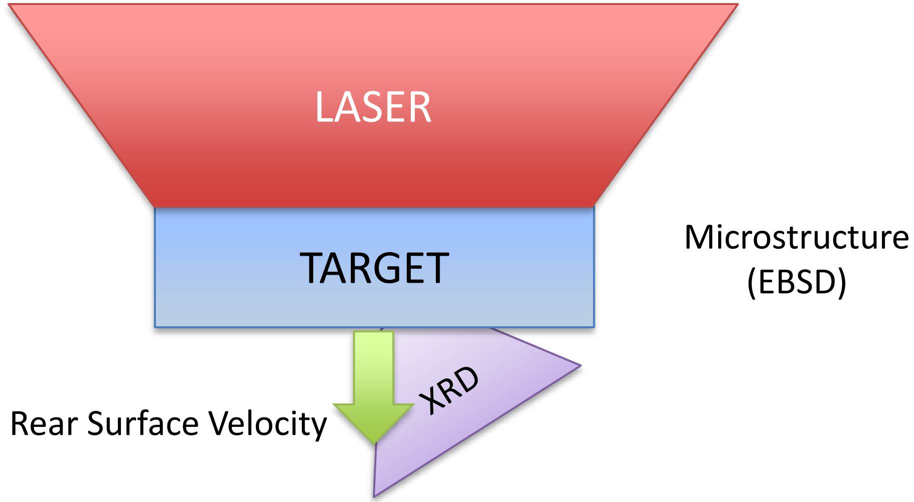
[D. D. Mallick et al. *Exp. Mech.* (2019)]



- Al flyer Thickness: 25 μm and 50 μm
- Laser Energy: up to 2 J; Spot size: 1.6 mm
- Pulse duration 10 ns

A Virtual Framework ….

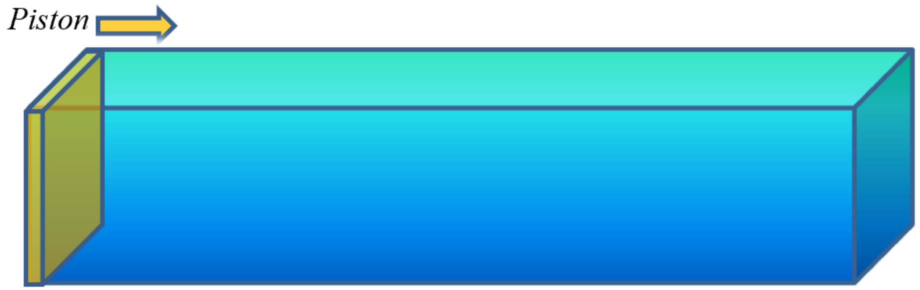




- XRD patterns to characterize twinning, phase transformation
- Characterize microstructure evolution to quantify twins and phase-transformed fractions
- Modeling the shock response at length scales and time scales of experiments
  - Sample thickness: 0.5µm to 50 µm
  - Shock pulse: up to 10 ns
- Modeling the laser-metal interaction to capture ablation/melting/shock generation
- XRD patterns under laser shock conditions
- Mesoscale modeling of laser shock experiments

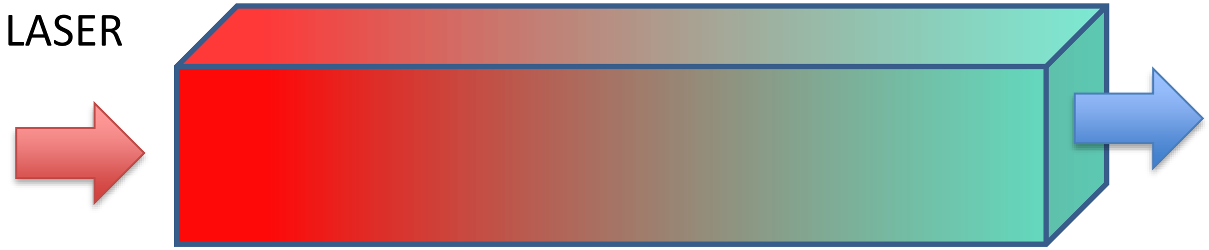
Our Approach

In Situ Diffraction Experiments (DCS)



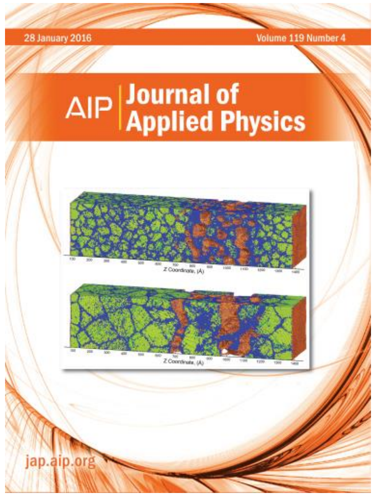
- **Atomic scale:** Molecular dynamics (shock/spall)
- **Virtual Diffraction (LAMMPS)**
- **Shock compression and release**
  - BCC (Fe)
- **Texture Analysis**
  - Phase/Twin Variant Selections
- **Mesoscale:** Quasi-Coarse-grained dynamics
  - Shock compression and release (BCC Fe)

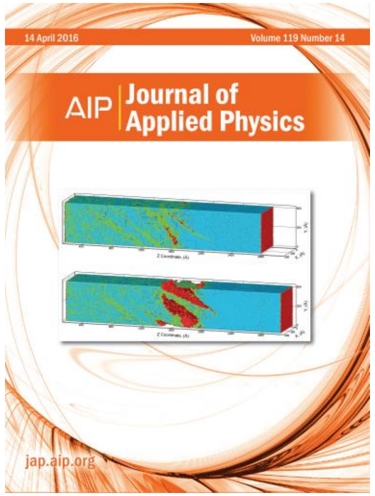
Laser-Driven Flyers (JHU)

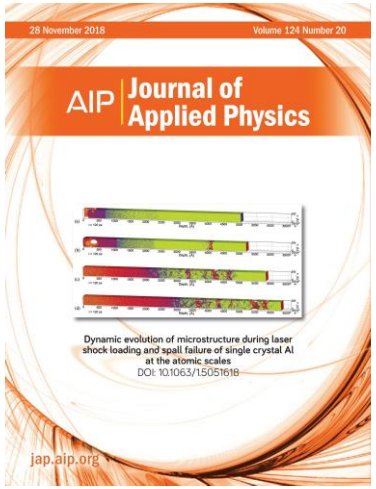


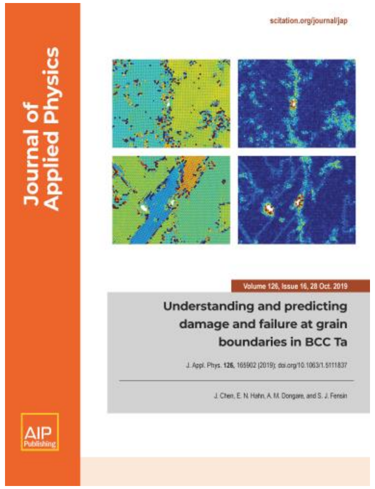
- **Atomistic-Continuum method:** Molecular dynamics + two-temperature method (MD-TTM)
- **Spall Failure**
  - FCC (Al), BCC (Ta)
- **Virtual Diffraction (LAMMPS)**
- **Mesoscale:** Quasi-Coarse-grained dynamics
  - Laser shock compression/spall failure
  - Laser-driven Flyers

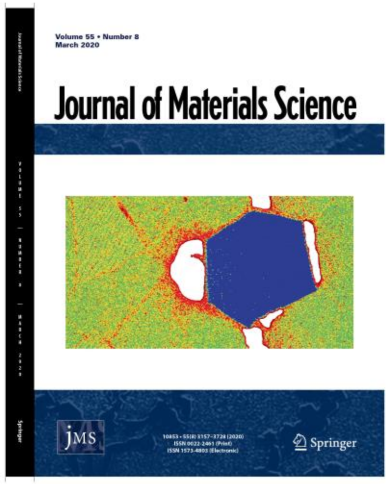
Molecular Dynamics to Understand Plasticity Mechanisms

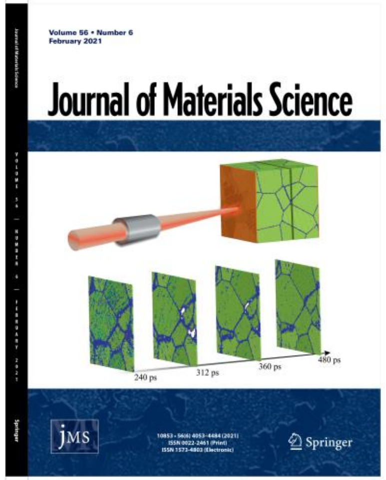










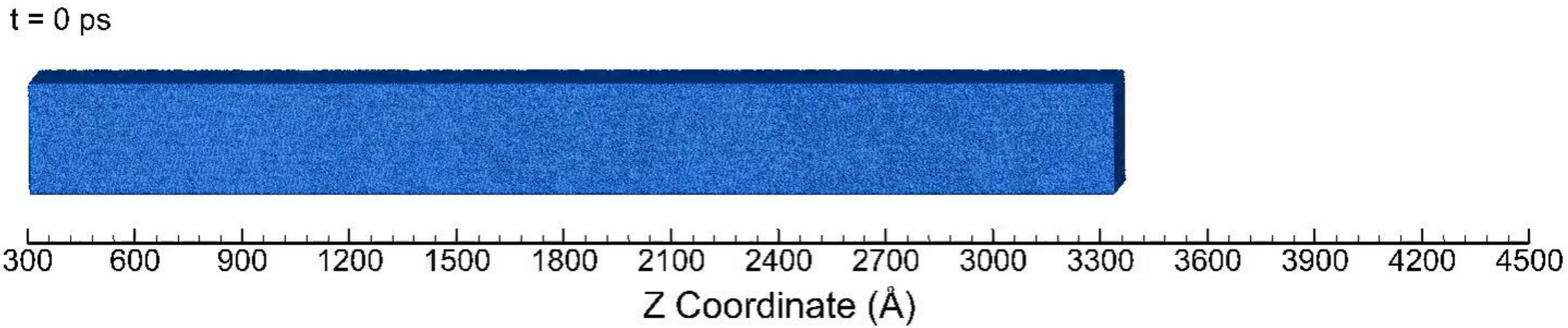


- **FCC**
  - Dongare et al., *Phys. Rev. B* 80, 10410 (2009)
  - Dongare et al., *J. Appl. Phys.* 108, 113518 (2010)
  - Mackenchery et al., *J. Appl. Phys.* 119, 044301 (2016)
  - Agarwal et al., *Comp. Mater. Sci.* 145, 68 (2018)
  - Valisetty et al., *Model. Simul. Mater. Sci. Eng.* 26, 055008 (2018)
  - Galitskiy et al., *J. Appl. Phys.* 124, 205901 (2018).
  - Valisetty et al., *Model. Simul. Mater. Sci. Eng.* 27, 065015 (2019)
  - Agarwal et al., *Int. J. Plasticity* 128, 102678 (2020).
  - Galitskiy et al., *J. Mater. Sci.* 56, 4446 (2021).
  - Ma et al., *J. Appl. Phys.* 129, 175901 (2021)
  - Echeverria et al., *Comp. Mater. Sci.* 198, 110668 (2021)

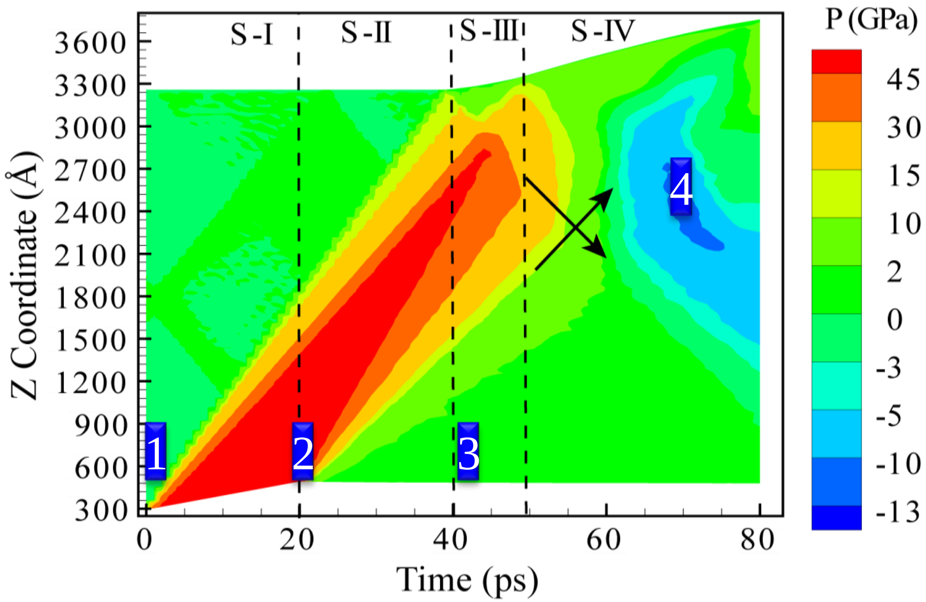
- **BCC:**
  - Chen et al., *J. Appl. Phys.* 126, 165902 (2019)
  - Mishra et al., *J. Appl. Phys.* 130, 215902 (2021).
  - Ma et al., *J. Mater. Sci.* 57, pages12556 (2022).

- **HCP:**
  - Agarwal et al., *J. Mater. Sci.* 52: 10853 (2017)
  - Agarwal et al., *Sci. Rep.* 9, 3550 (2019).
  - Flanagan et al., *Materials & Design* 194: 108884 (2020)

MD: Spall Failure of Fe (110)

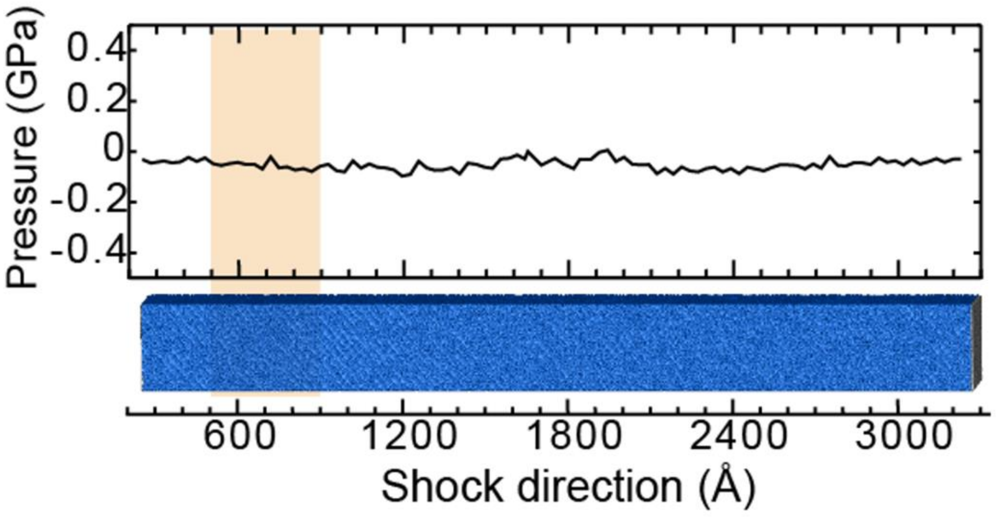


- **Microstructure:** Single-crystal Fe (110)
- **Impact velocity:** 1 km/s
- **Interatomic potential:** EAM [Gunkelmann, PRB (2012)]
- **Shock pressure:** ~ 85 GPa
- **Virtual XRD characterization using LAMMPS**

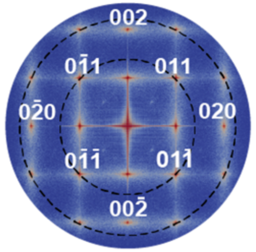


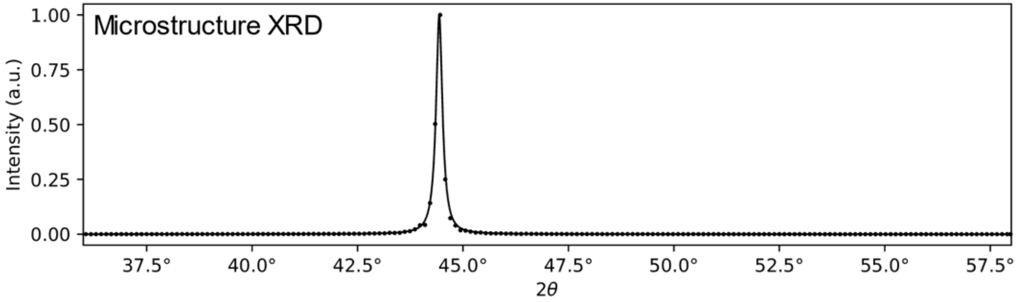
[Mishra et al., *Sci. Rep.* (2021)]

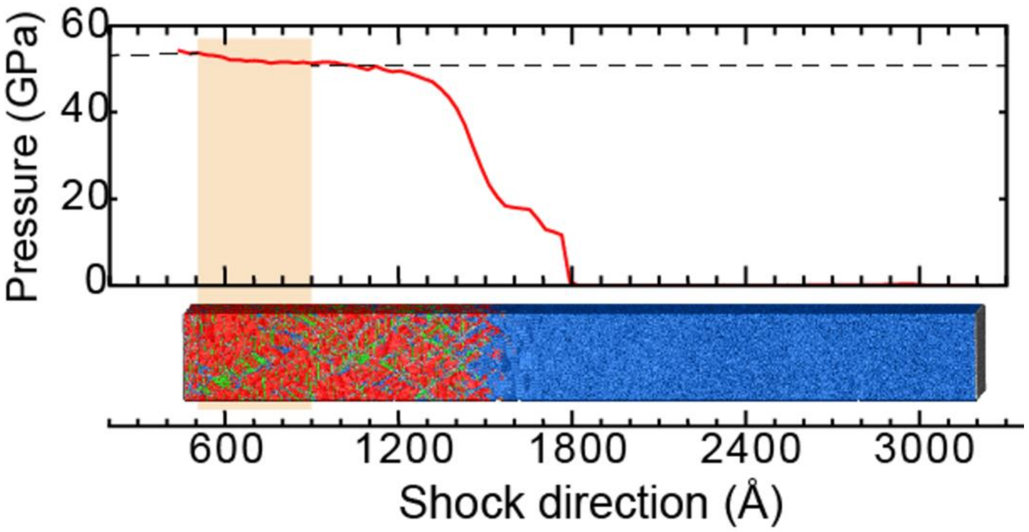
Virtual XRD: Shock Compression - Fe (110)



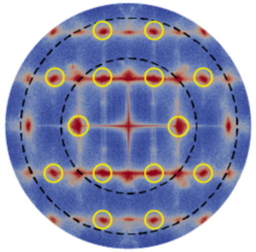
Initial System: 100 % BCC

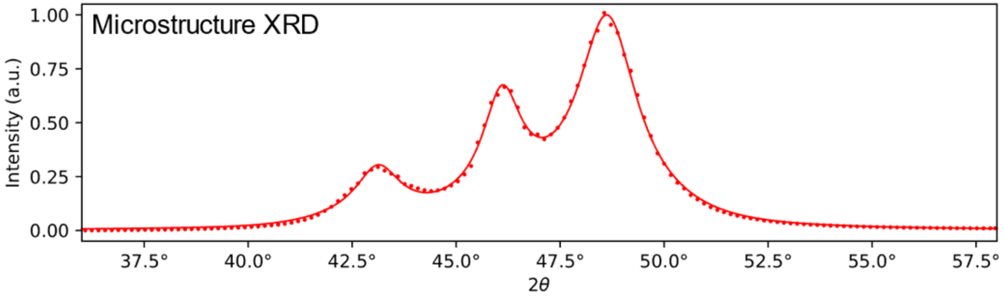




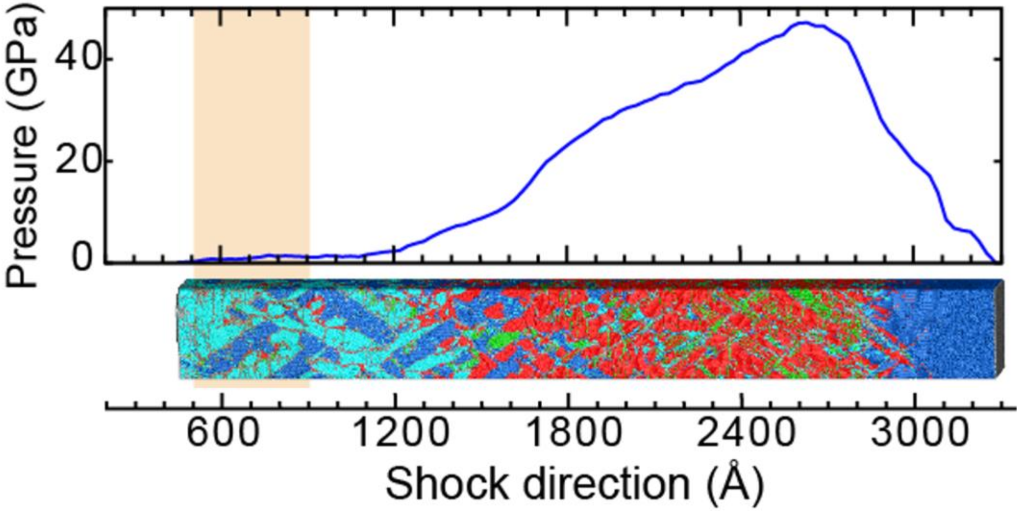


Shock-compressed: ~8 % BCC, 67 % HCP, 11% FCC

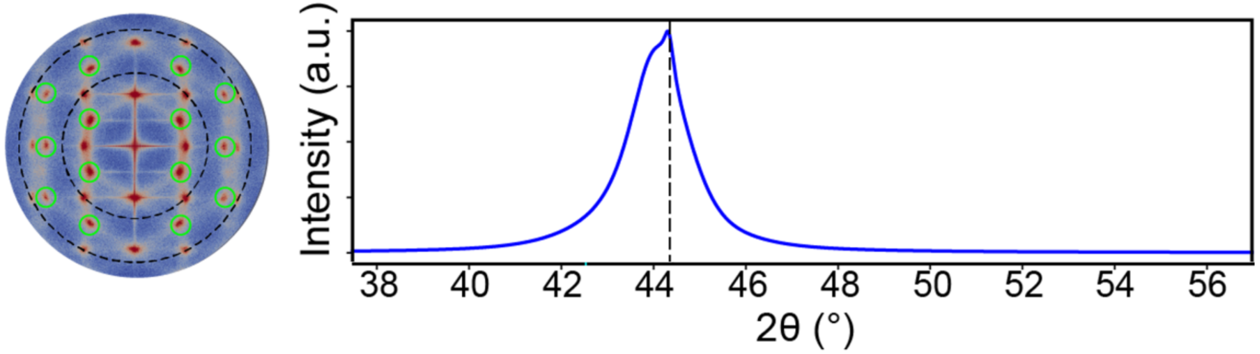


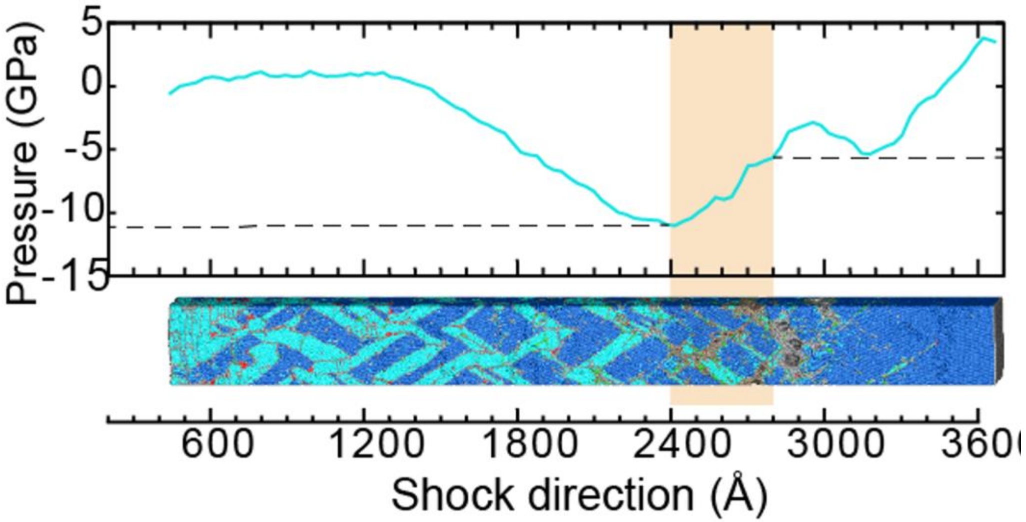


Virtual XRD: Shock Release and Spall Failure - Fe (110)

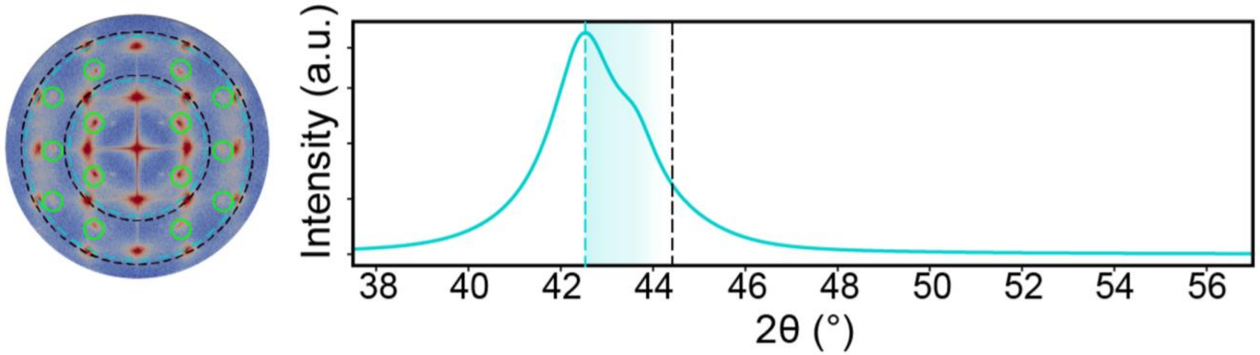


Shock release: 71% BCC (46% twins), 4% HCP, and 1% FCC





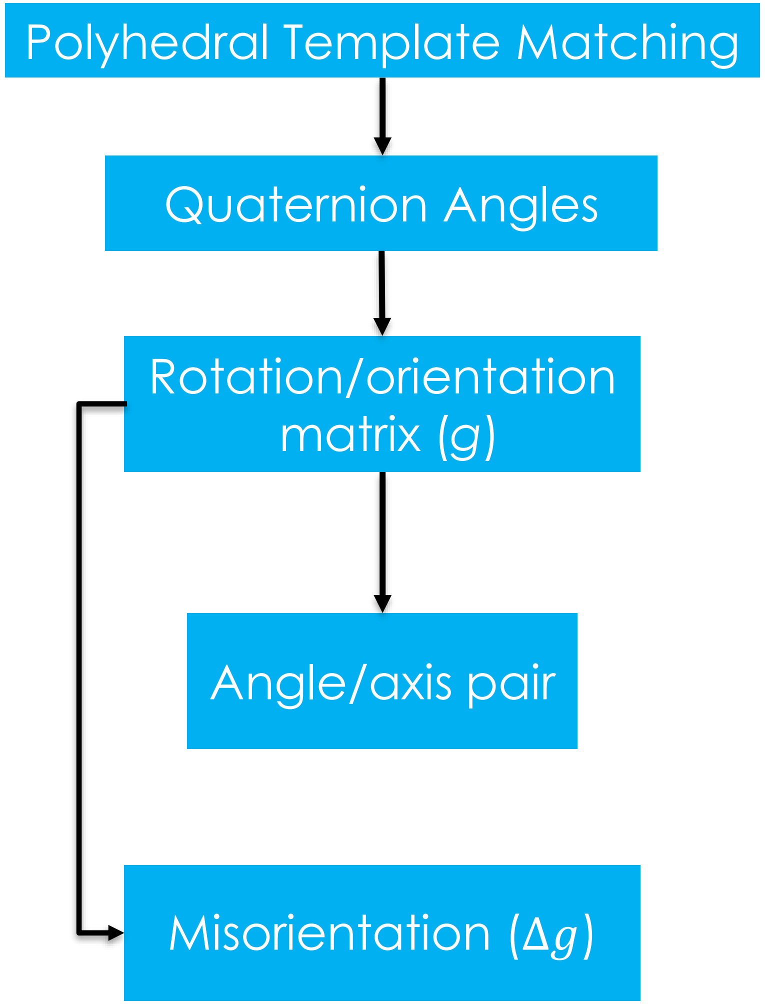
Spall Failure: 64% BCC (46% twins), 1% HCP, and 3% FCC



[Mishra et al., *Sci. Rep.* (2021)]

Virtual Texture Analysis (VirTex): Virtual EBSD

- A tool for texture analysis of atomistic microstructures to identify phase and twin variants



Polyhedral Template Matching

Quaternion Angles

Rotation/orientation matrix (g)

Angle/axis pair

Misorientation (Δg)

Quaternions: $(q_x\ q_y\ q_z\ q_w)$

$$g = \begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$$

$$g = \begin{bmatrix} 1 - 2(q_y^2 + q_z^2) & 2(q_x q_y - q_z q_w) & 2(q_x q_z + q_y q_w) \\ 2(q_x q_y + q_z q_w) & 1 - 2(q_x^2 + q_z^2) & 2(q_y q_z - q_z q_w) \\ 2(q_x q_z - q_y q_w) & 2(q_y q_z + q_x q_w) & 1 - 2(q_x^2 + q_y^2) \end{bmatrix}$$

$$\theta = \cos^{-1}\left(\frac{g_{11} + g_{22} + g_{33} - 1}{2}\right)$$

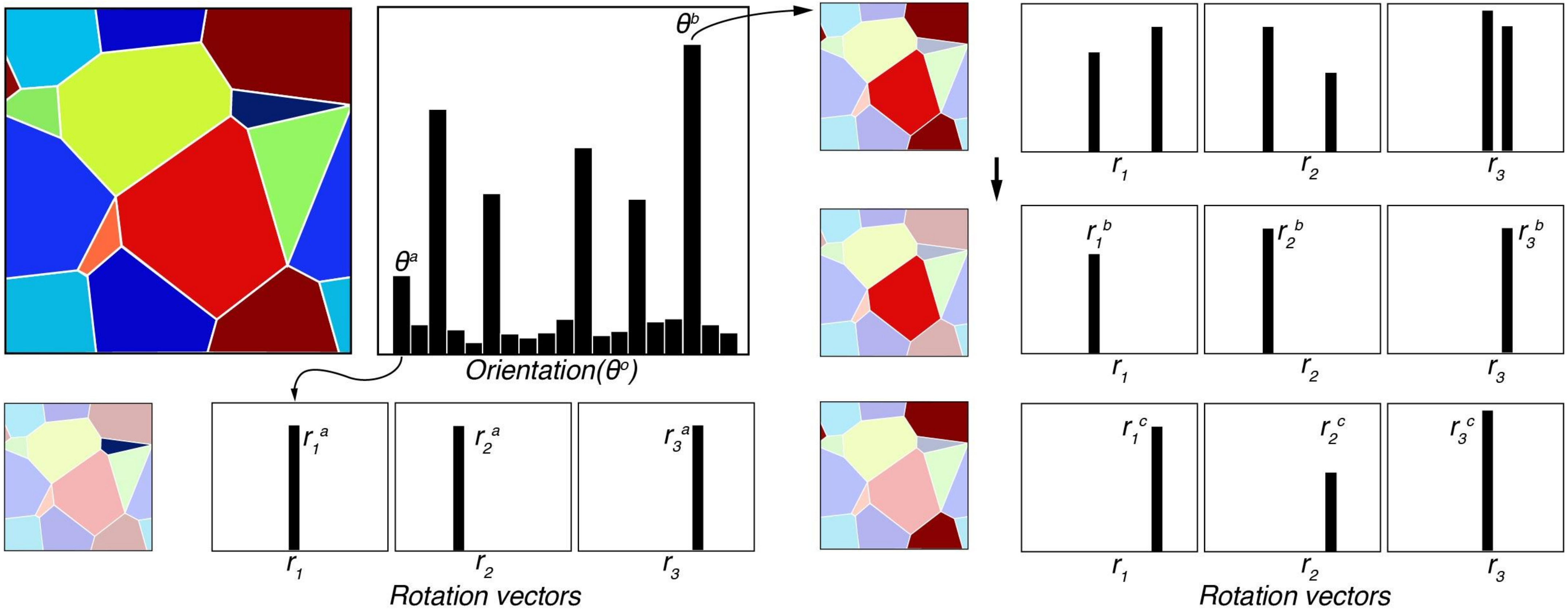
$$r_1 = \left(\frac{g_{23} - g_{32}}{2Sin\theta}\right), r_2 = \left(\frac{g_{31} - g_{13}}{2Sin\theta}\right), r_3 = \left(\frac{g_{12} - g_{21}}{2Sin\theta}\right),$$

$$\Delta g = g_1 . g_2^{-1} \qquad \Theta = \cos^{-1}\left(\frac{\Delta g_{11} + \Delta g_{22} + \Delta g_{33} - 1}{2}\right)$$

[Mishra et. al, *J. Mater. Sci.* (2022)]

Virtual Texture Analysis (VirTex)

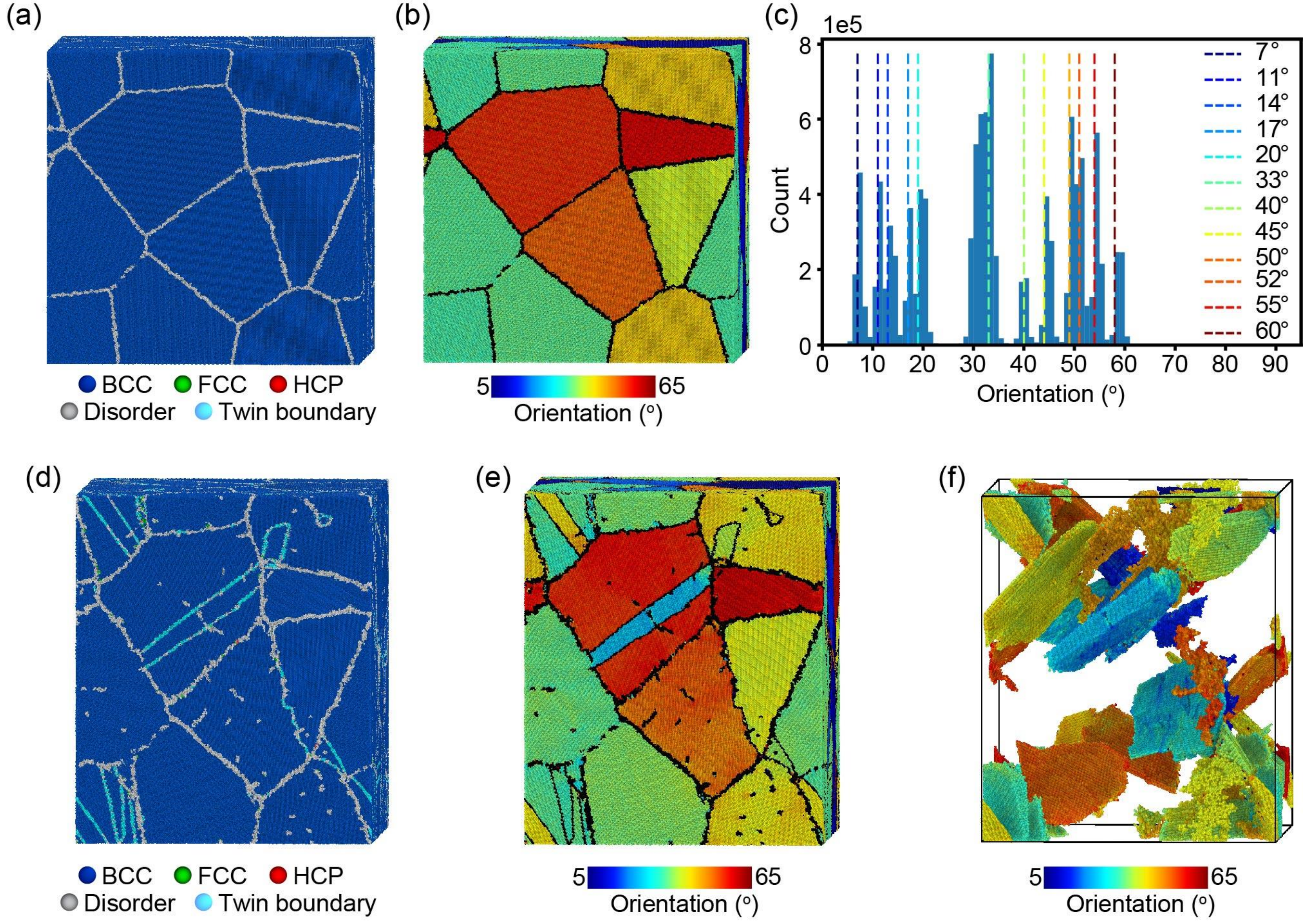
- A unique set of angle/axis pairs is determined to identify grain, phase, twins, and their variants



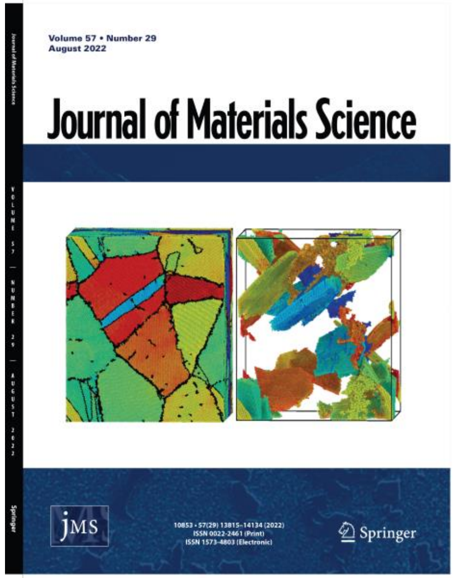
- Automatic peak identification from histograms and determination of unique set of angle/axis pairs

[Mishra et. al, *J. Mater. Sci.* (2022)]

Variant Selections during Compression in Ta



- VirTEX: Characterize twin/phase variants in deformed microstructures generated using MD simulations.


Volume 57 • Number 29
August 2022

Journal of Materials Science

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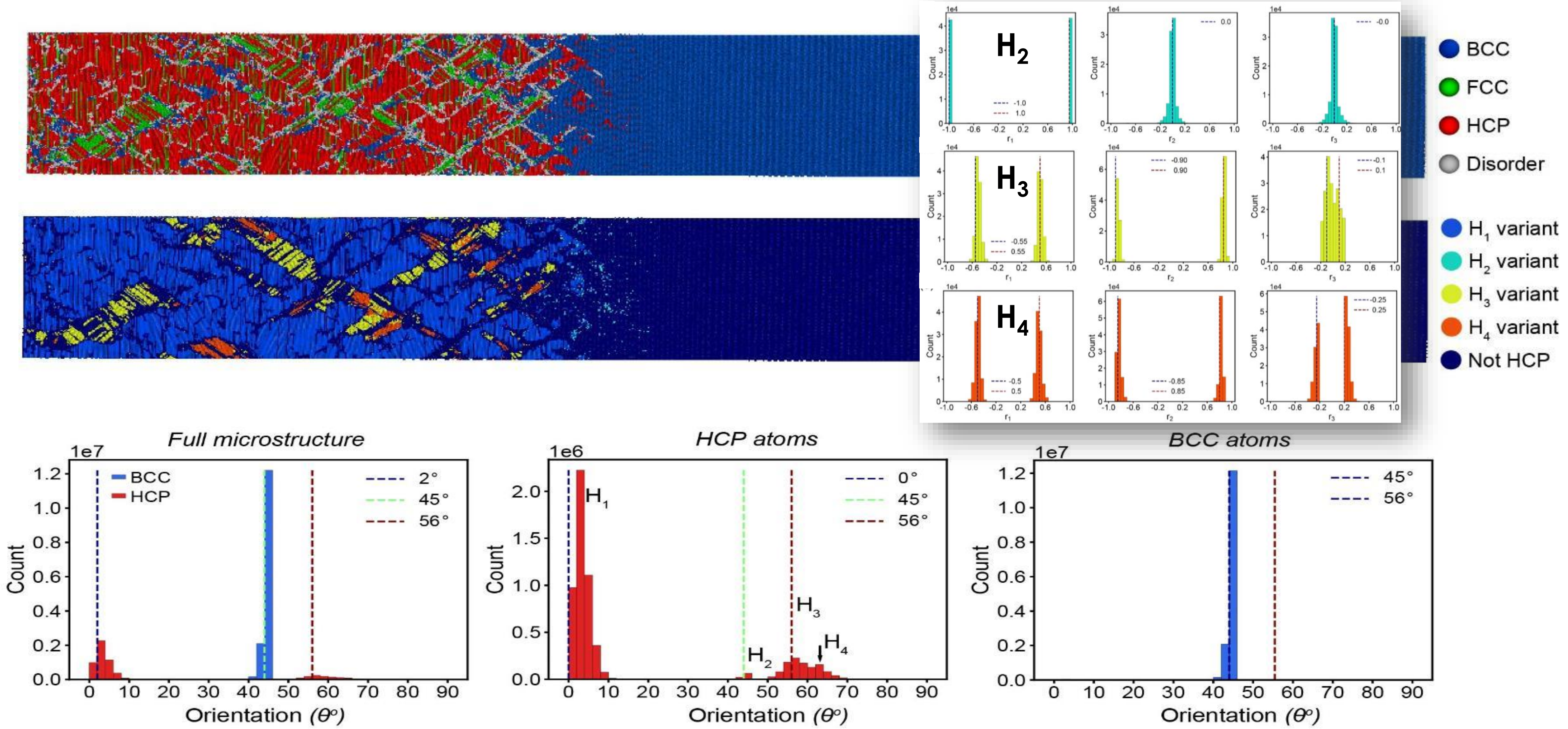
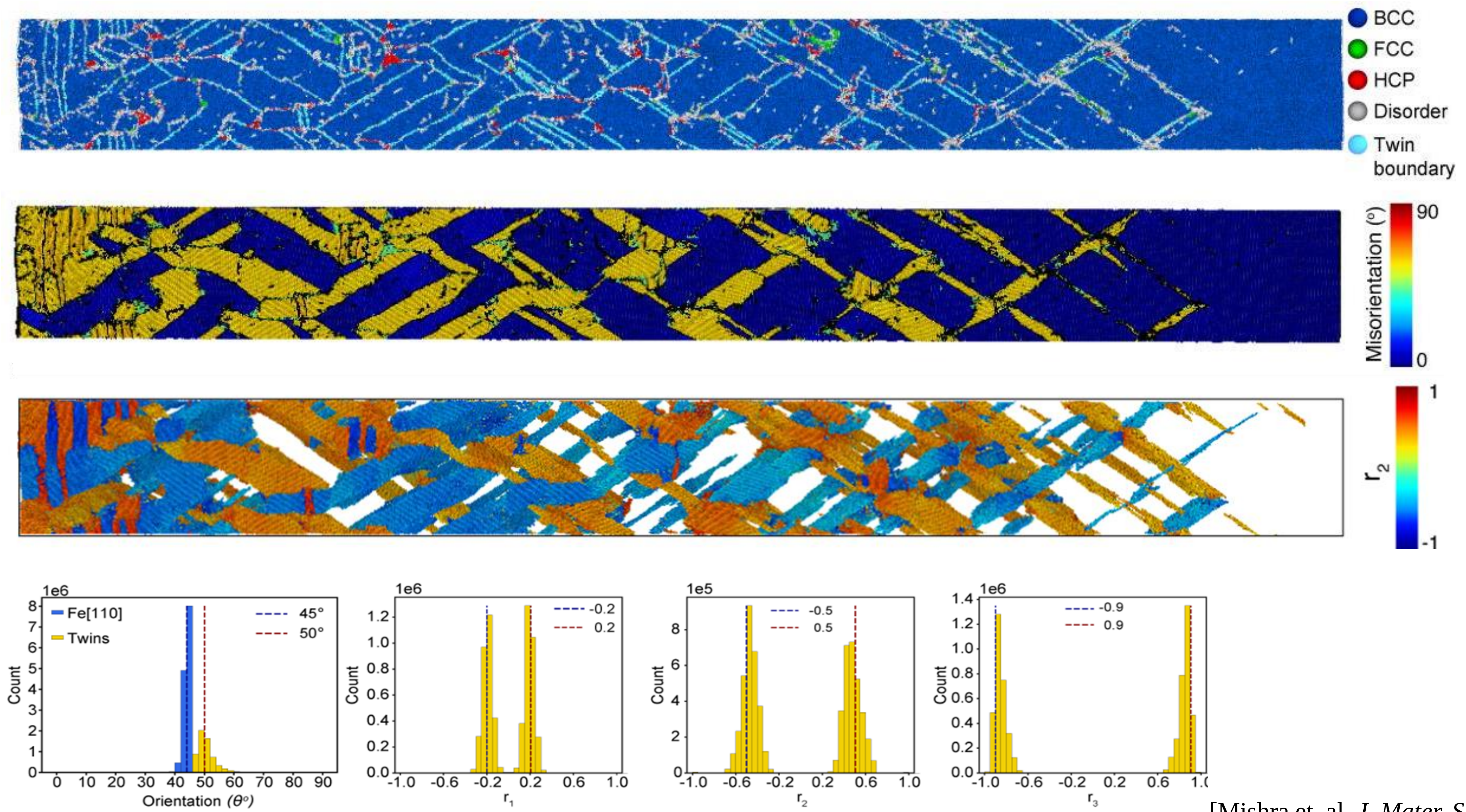
[Mishra et. al, *J. Mater. Sci.* (2022)]

Variant Selections during $\alpha \rightarrow \varepsilon$ HCP Phase Transformation in [110] Fe



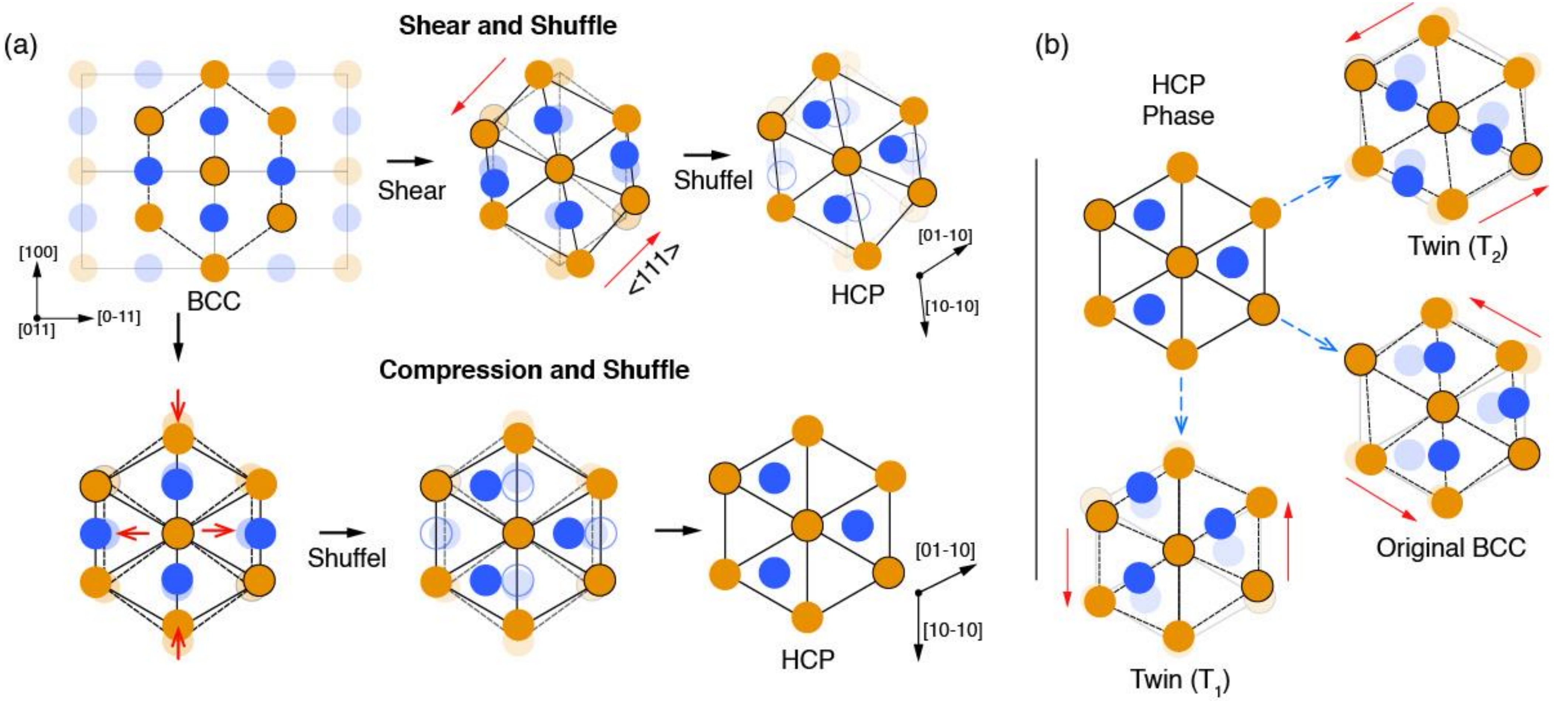
[Mishra et. al, *J. Mater. Sci.* (2022)]

Variant Selections during $\varepsilon \rightarrow \alpha$ Phase Transformation in [110] Fe



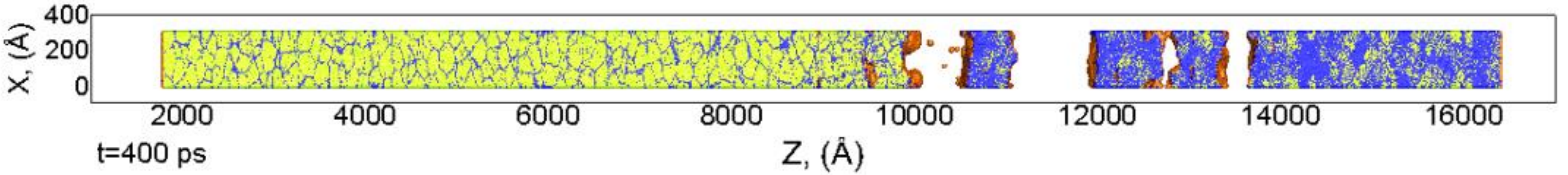
[Mishra et. al, *J. Mater. Sci.* (2022)]

$\alpha \rightarrow \varepsilon \rightarrow \alpha$ Phase Transformation in Fe



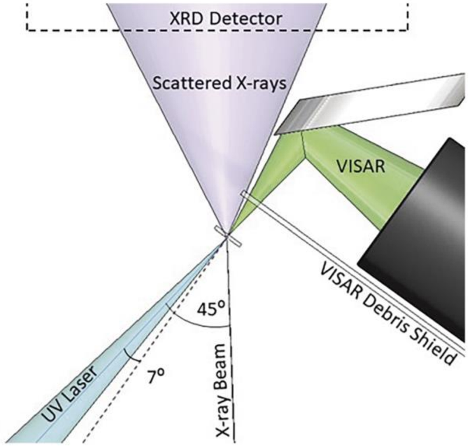
$\alpha \rightarrow \varepsilon \rightarrow \alpha$ follows the Burgers pathway model: The orientation relationships allow 12 different HCP variants from a single BCC phase orientation. The symmetries in the HCP phase allow six BCC variants upon reverse phase transformation, two of which are twinning variants.

MD Simulations: Time and Length Scale Challenges



- Mechanisms of nucleation and evolution of defects/damage is a challenge
- **MD Simulations limited to small system sizes** (100s of nm) and short simulation times (up to a few tens of ps) for shock loading
- **Big-data Challenge:** post-processing of very large data sets (TBs)
- *In situ* diffraction experiments have samples with dimensions ranging from **1-50 microns** and **wave propagation times of up to 10 ns**

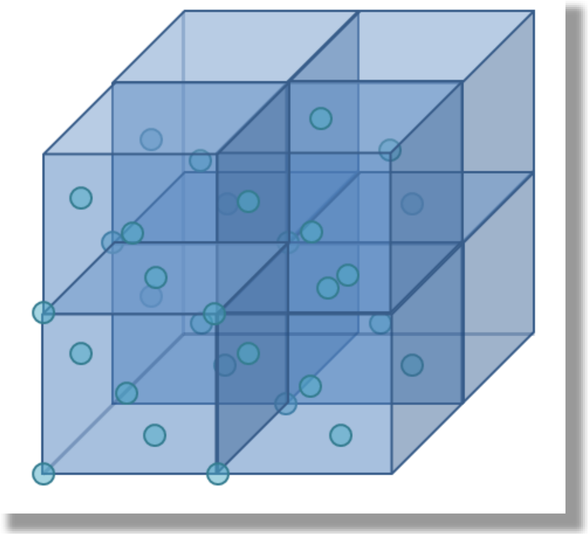
In situ diffraction

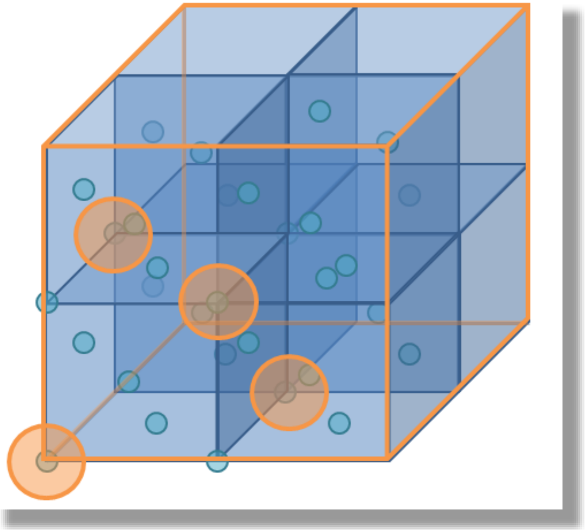


[Wang et al., Rev. Sci. Instrum. (2019)]

Mesoscale models to replicate length/time scales of *in situ* shock experiments

Mesoscale Modeling: Quasi-Coarse-Grained Dynamics





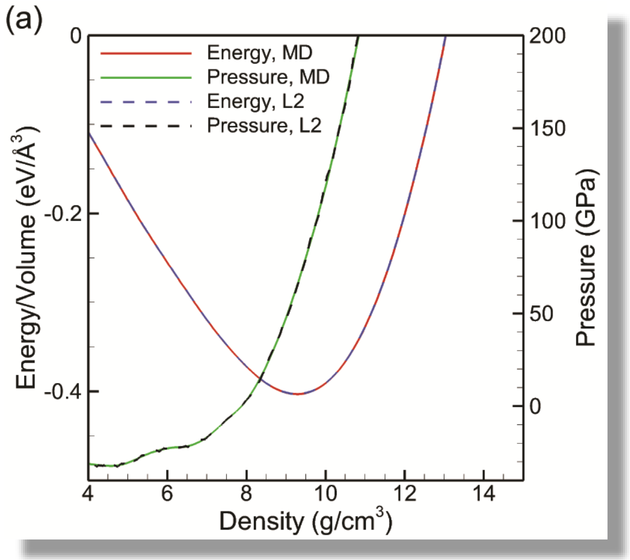
- Coarse graining the structure using representative atoms (R-atoms) and retain the crystal structure orientation relationships and symmetry

- MD Energy of each R-atom retained by scaling bond lengths in the interatomic potential

$$E_i^R = \frac{1}{2}\sum_{j\neq i}\varphi_{ij}\left(\frac{r_{ij}^R}{A_{cg}}\right) + F_i\left[\sum_{j\neq i} f_j\left(\frac{r_{ij}^R}{A_{cg}}\right)\right]$$

Distance scaling: A_{cg}

No. of Atoms scaling: N_{cg}



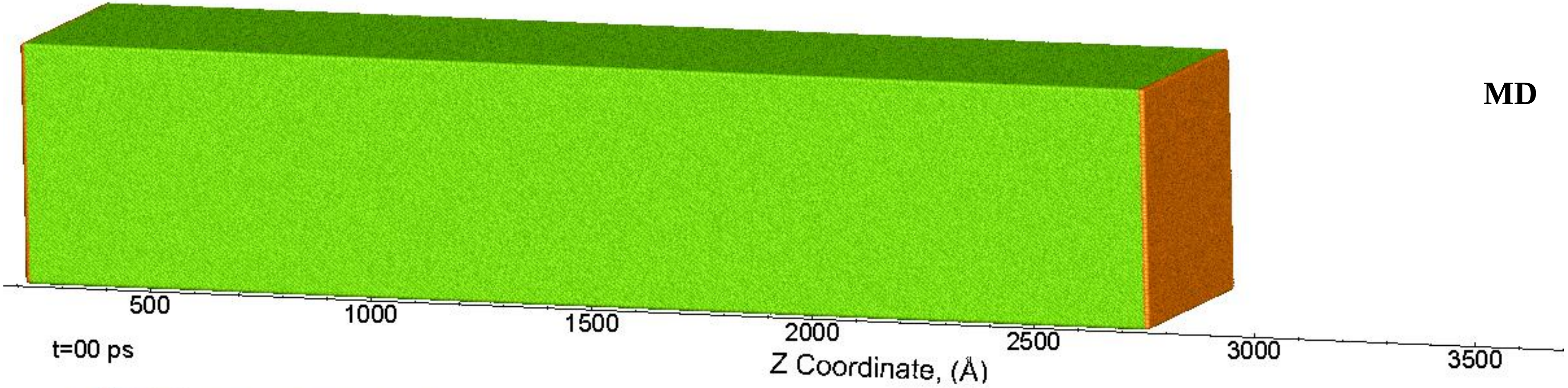
- The energy of each R-atom is scaled to account for missing atoms

→ **L2**: 2x2x2 unit cells → 1 CG cell; $A_{cg} = 2$; $N_{cg} = 8$

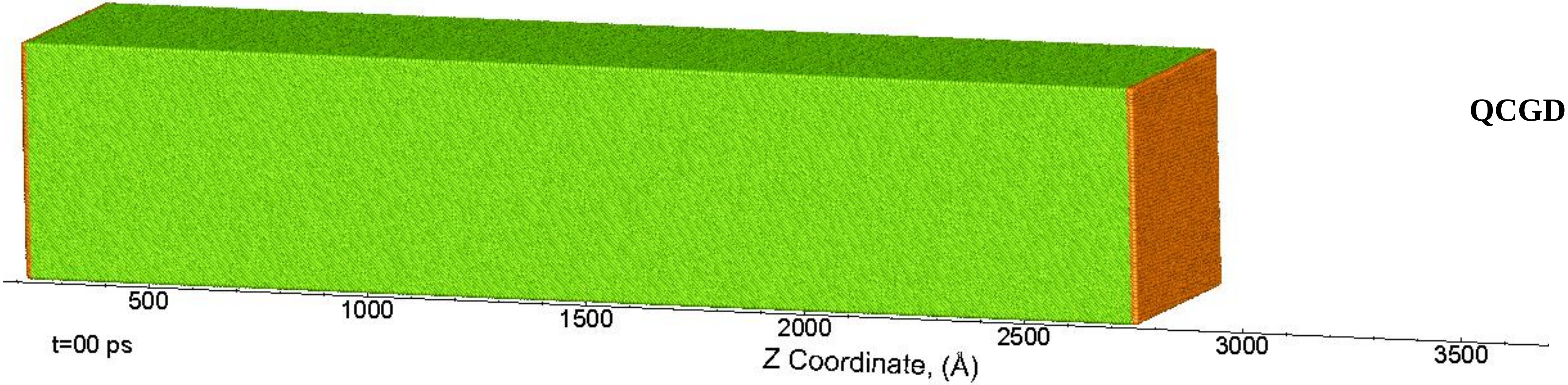
→ **L4:** 4x4x4 unit cells → 1 CG cell; $A_{cg} = 4$; $N_{cg} = 64$

[A. M. Dongare, *Phil. Mag.* **94**, 3877 (2014)]

Single Crystal Al (001) Spall Failure: MD vs L2-QCGD



MD

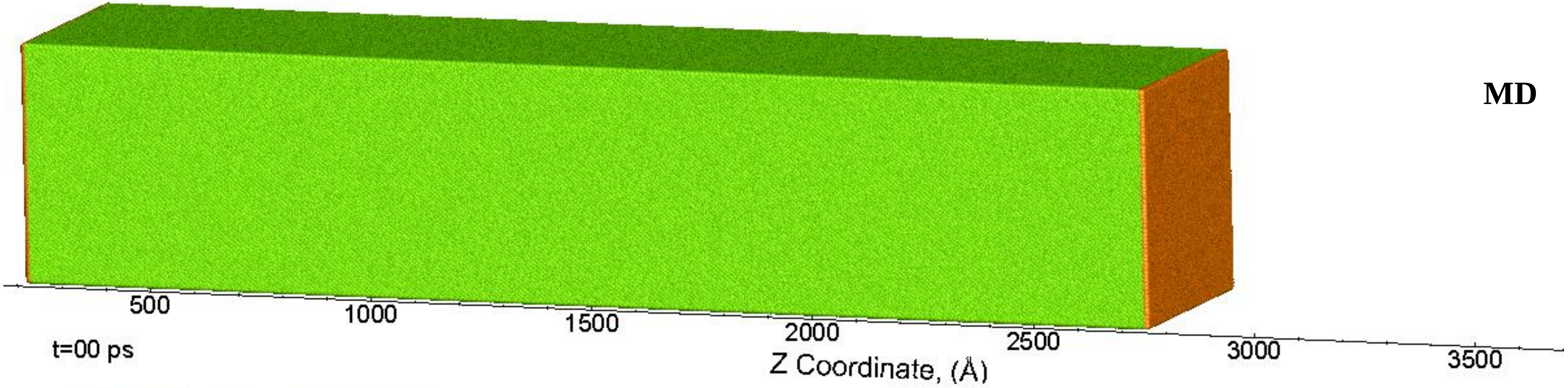


QCGD

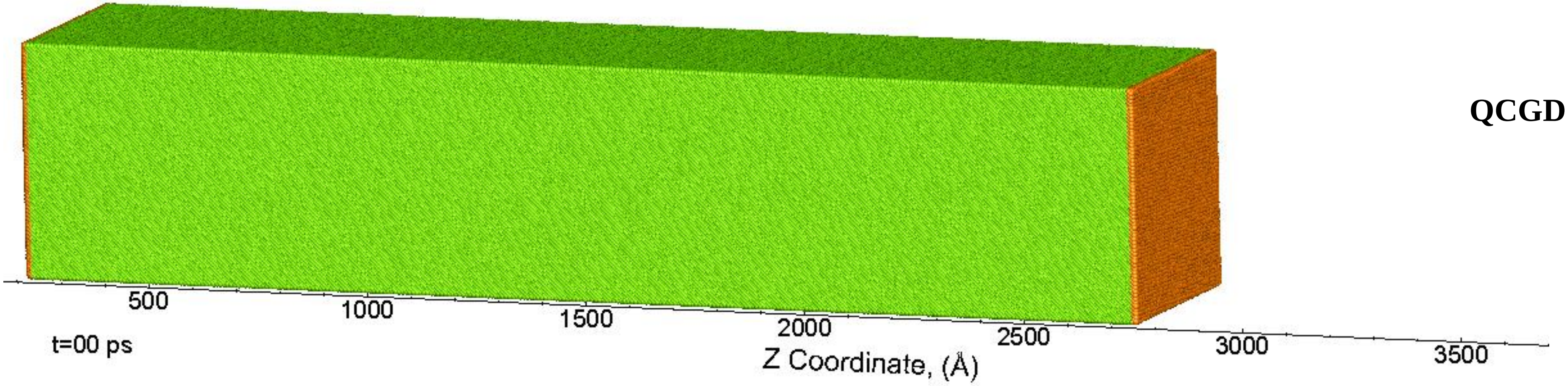
🟩 FCC 🟨 Twin faults 🟧 Surface 🟦 Disordered 🟦 Twin partials

[Agarwal and Dongare, *Comp. Mater. Sci.* **145**, 68 (2018)]

Single Crystal Al (001) Spall Failure: MD vs L2-QCGD



MD

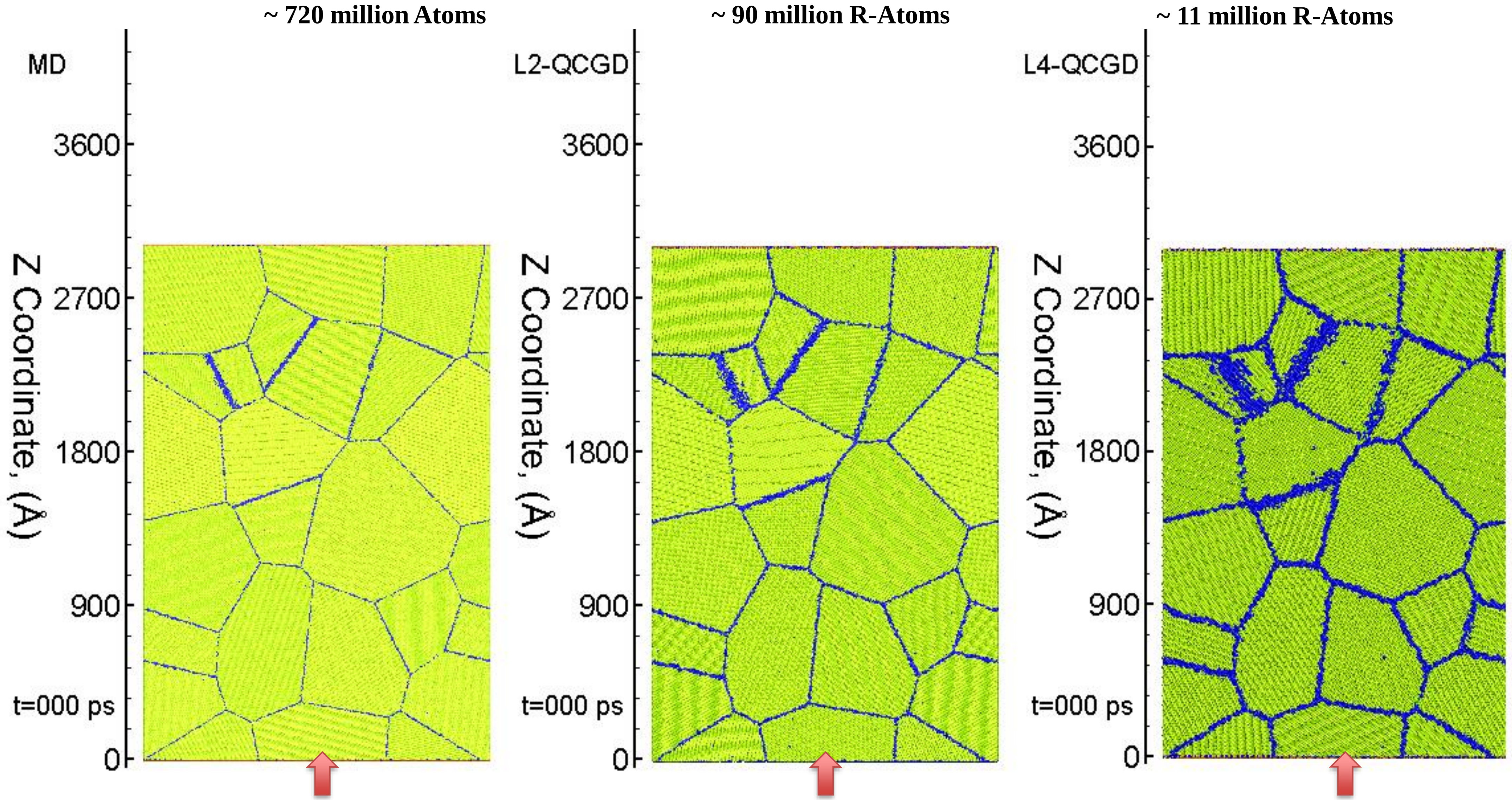


QCGD

🟩 FCC 🟨 Twin faults 🟧 Surface 🟦 Disordered ■ Twin partials

[Agarwal and Dongare, *Comp. Mater. Sci.* **145**, 68 (2018)]

Polycrystalline Al: MD vs QCGD-L2 vs QCGD-L4



🟨 **FCC** 🟩 **Stacking fault** 🟦 **Disordered** 🟧 **Surface**

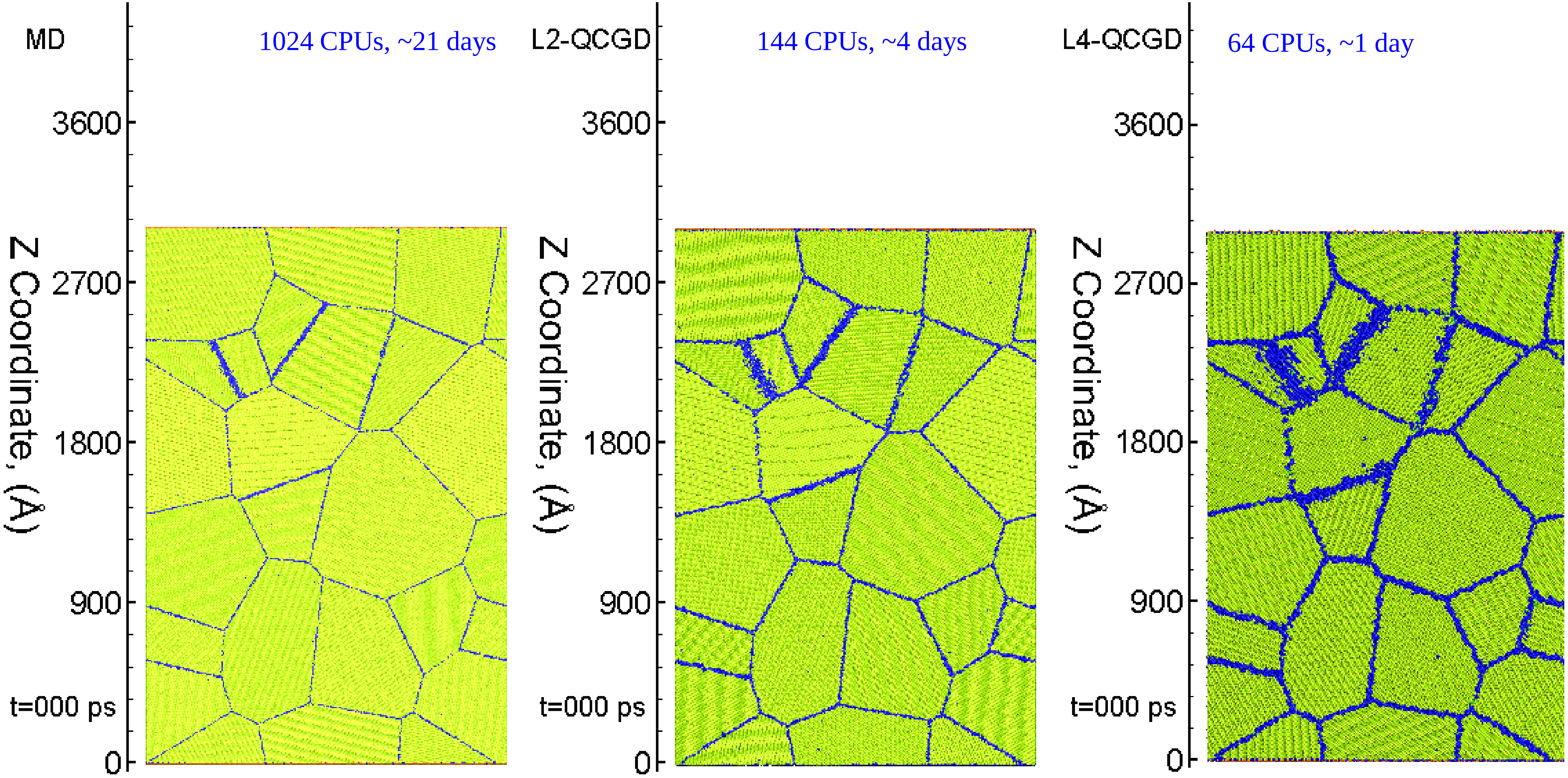
[Agarwal and Dongare, *IJP* (2020)]

Polycrystalline Al: MD vs QCGD-L2 vs QCGD-L4

~ 720 million Atoms

~ 90 million R-Atoms

~ 11 million R-Atoms



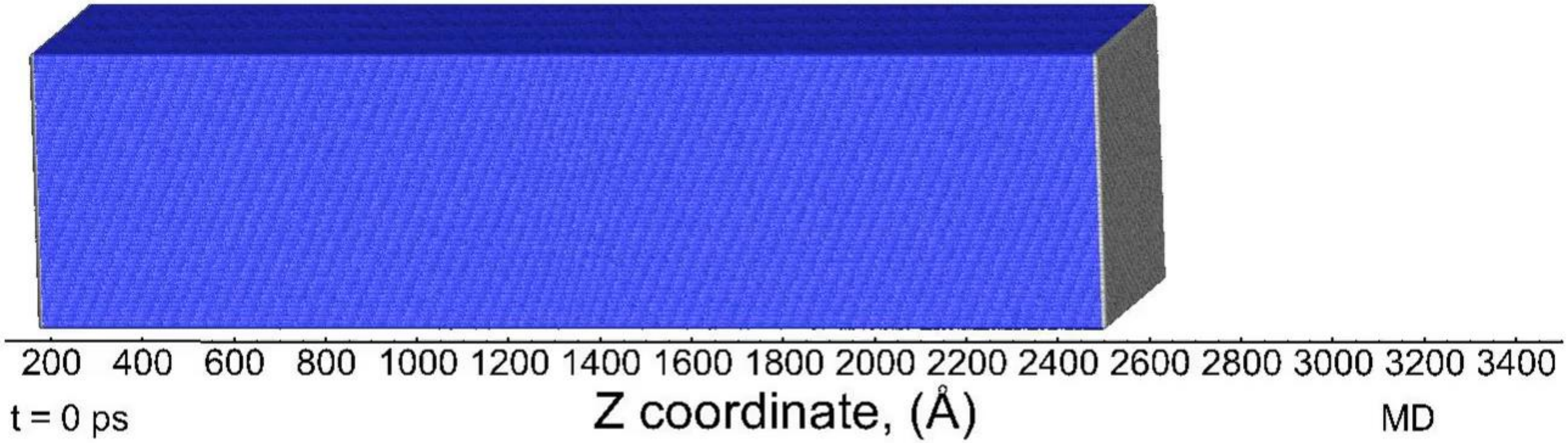
🟨 **FCC** 🟩 **Stacking fault** 🟦 **Disordered** 🟧 **Surface**

[Agarwal and Dongare, *IJP* (2020)]

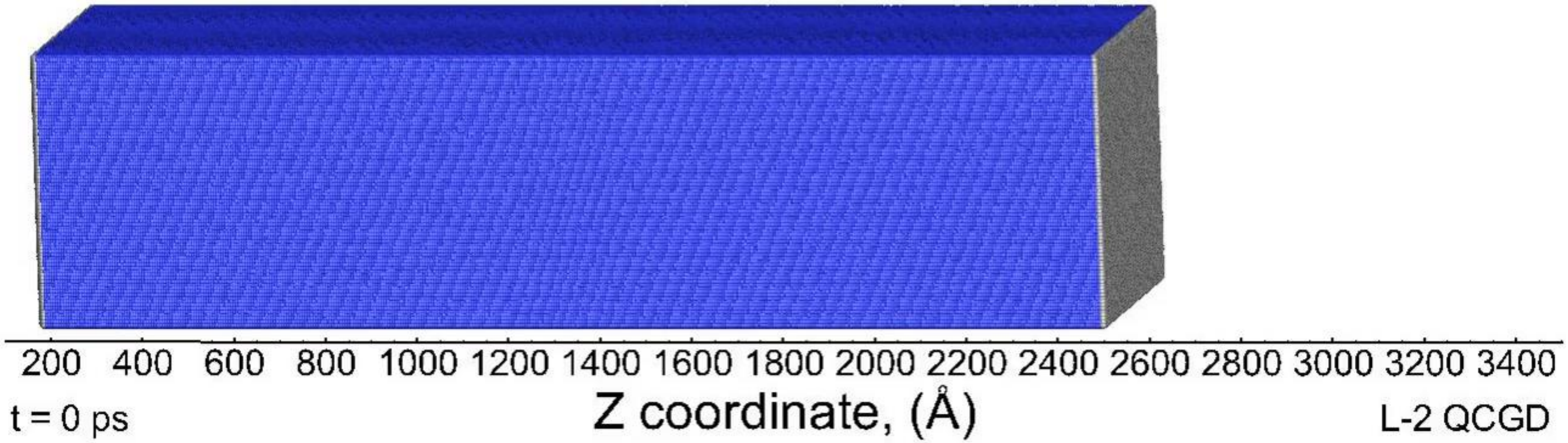
Single Crystal Fe (001) Spall Failure: MD vs L2-QCGD

HCP BCC

FCC OTHER



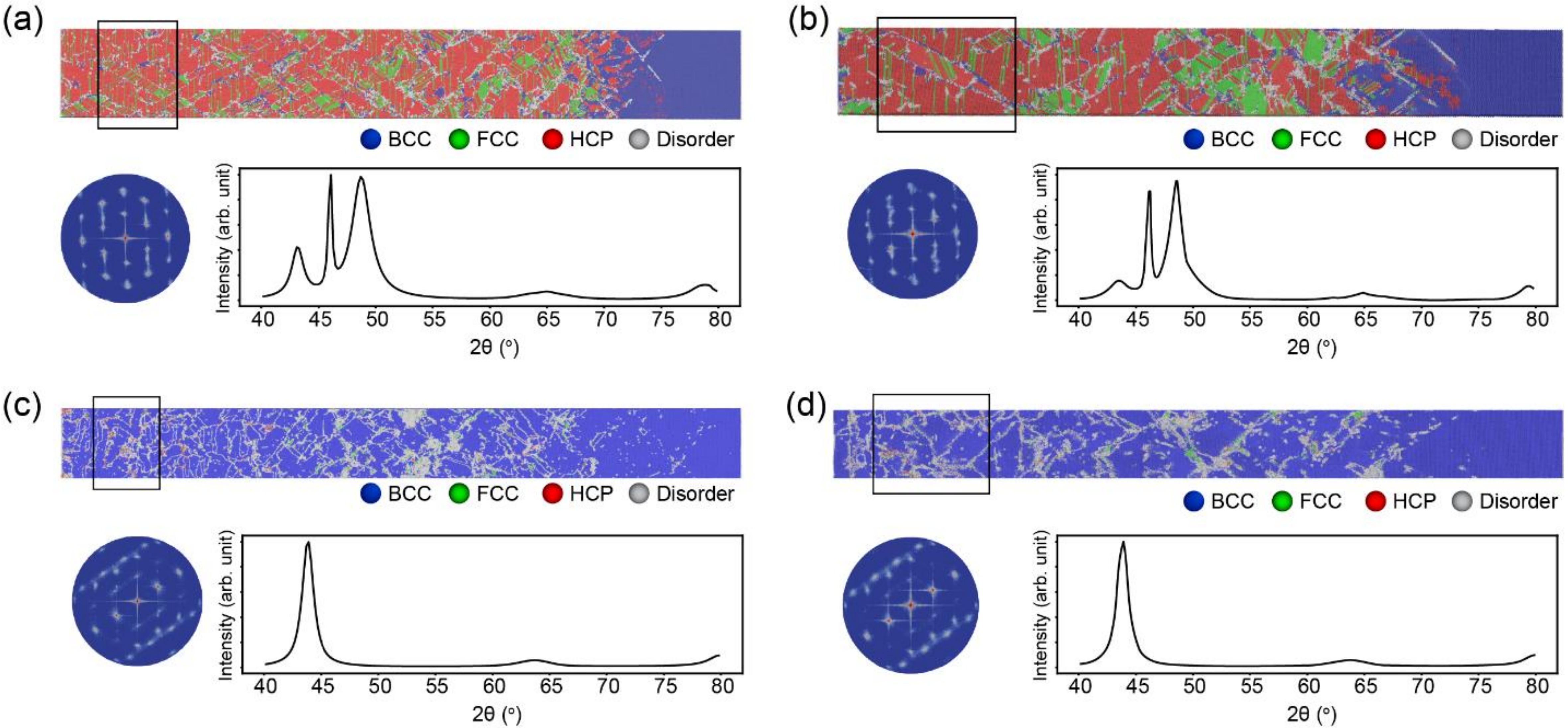
MD: ~ 40M atoms



L2: ~ 5M R-atoms

[Ma and Dongare, *J. Mater. Sci.* (in preparation)]

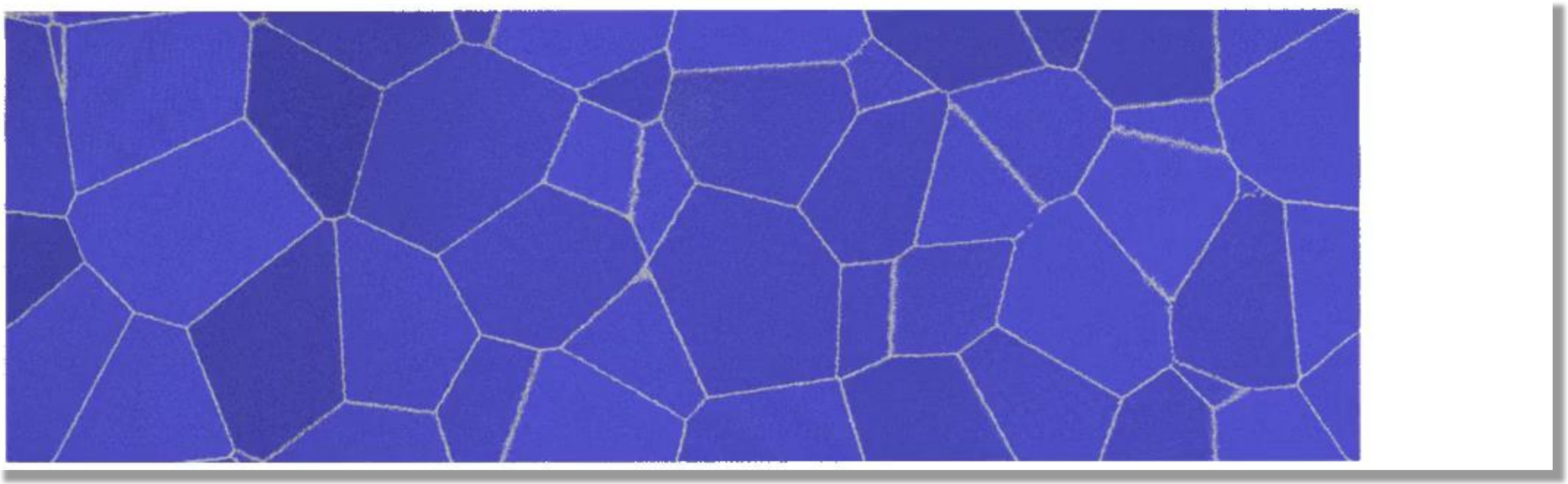
Fe [110] Shock Compression/Release: MD vs. QCGD



[Mishra et. al, J. Mater. Sci. 57, 12782 (2022)]

$\alpha \rightarrow \varepsilon \rightarrow \alpha$ Phase Transformation in Polycrystalline Fe

QCGD (8 µm x 8 µm x 25 µm): ~ 400M atoms

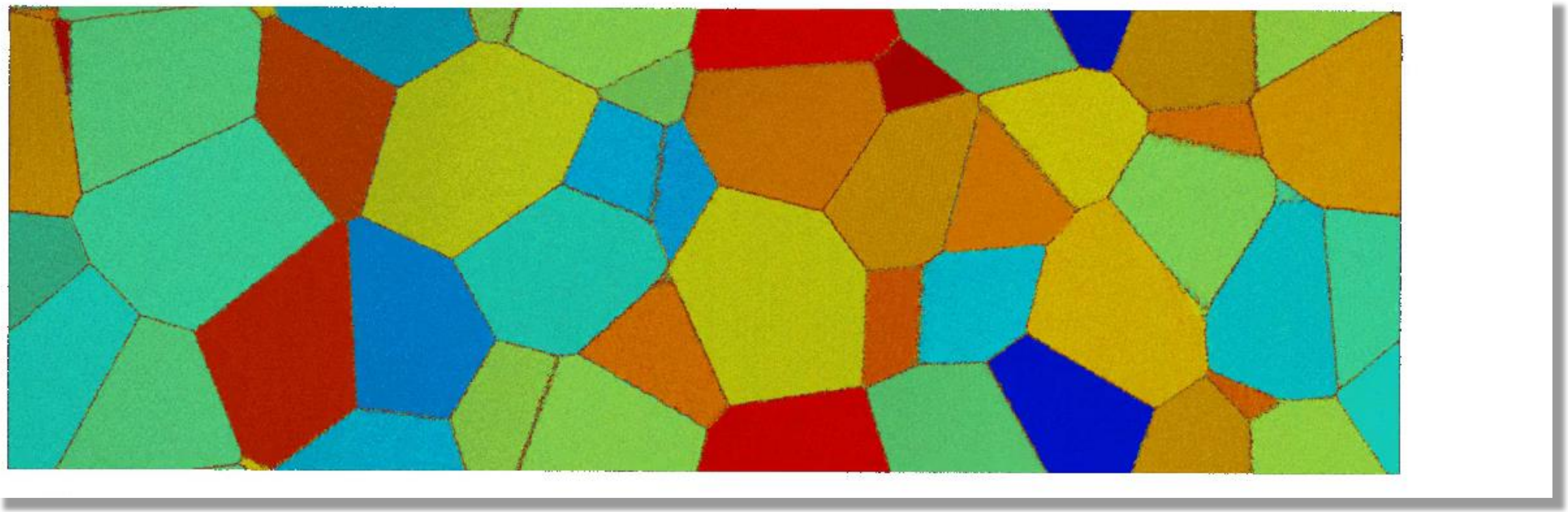


HCP **BCC** **FCC** **OTHER**

- Polycrystalline Fe shocked to $\alpha \rightarrow \varepsilon \rightarrow \alpha$ Phase Transformation during shock compression and release

$\alpha \rightarrow \varepsilon \rightarrow \alpha$ Phase Transformation in Polycrystalline Fe

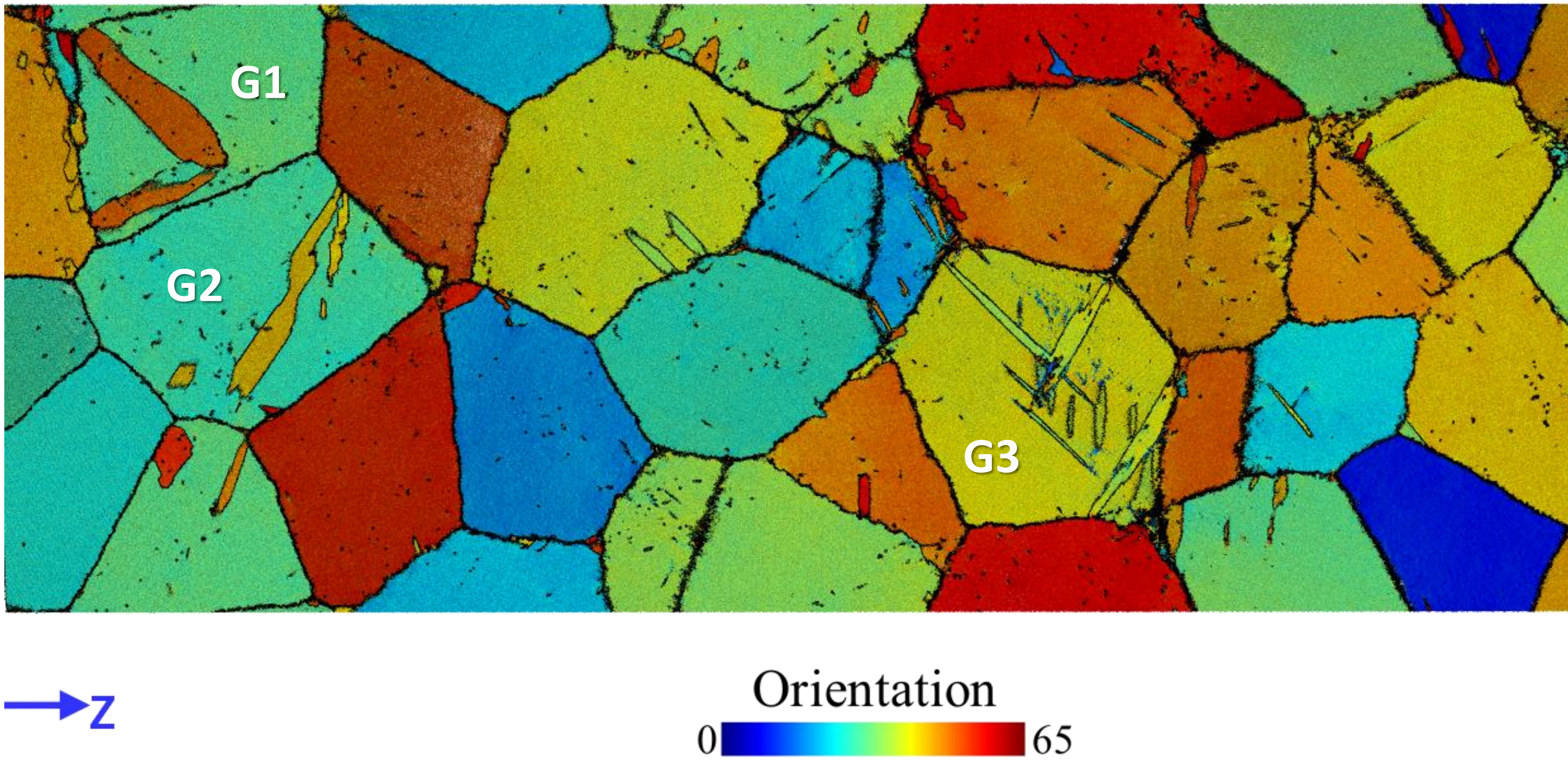
QCGD (8 µm x 8 µm x 25 µm): ~ 400M atoms

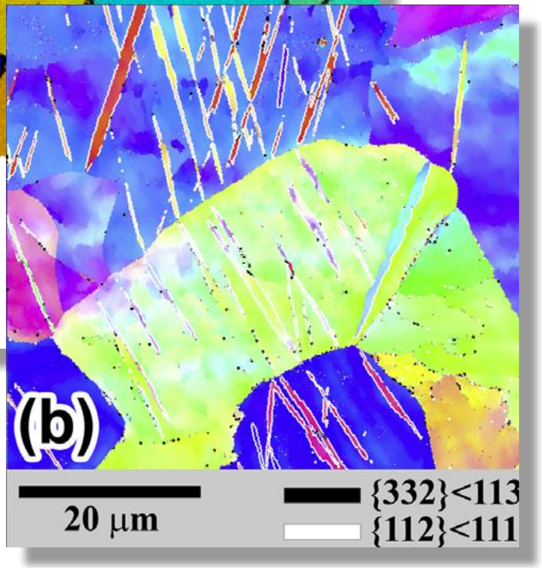


- Polycrystalline Fe shocked to $\alpha \rightarrow \varepsilon \rightarrow \alpha$ Phase Transformation during shock compression and release

0 **65** Orientation

$\alpha \rightarrow \varepsilon \rightarrow \alpha$ Shock-Recovered Polycrystalline Fe Microstructure



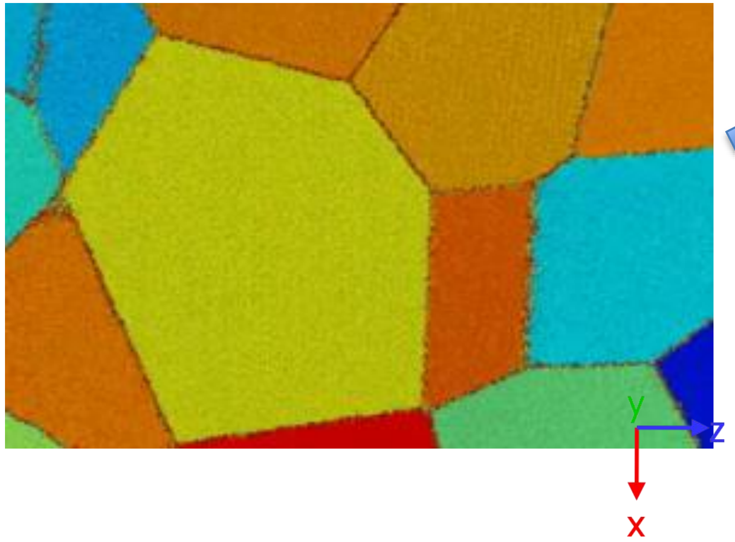


[Dougherty, et al., Scripta Mater. (2009)]

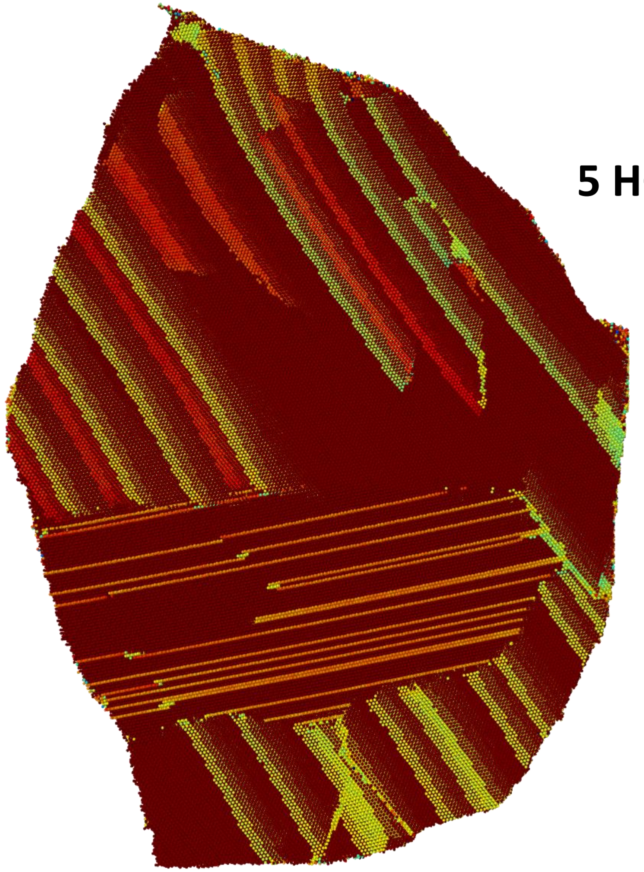
Twin structures during shock release are determined by loading orientations

Variant Selections in Individual Grains: G3

- Phase $\alpha \rightarrow \varepsilon$ transformation initiates at grain boundaries



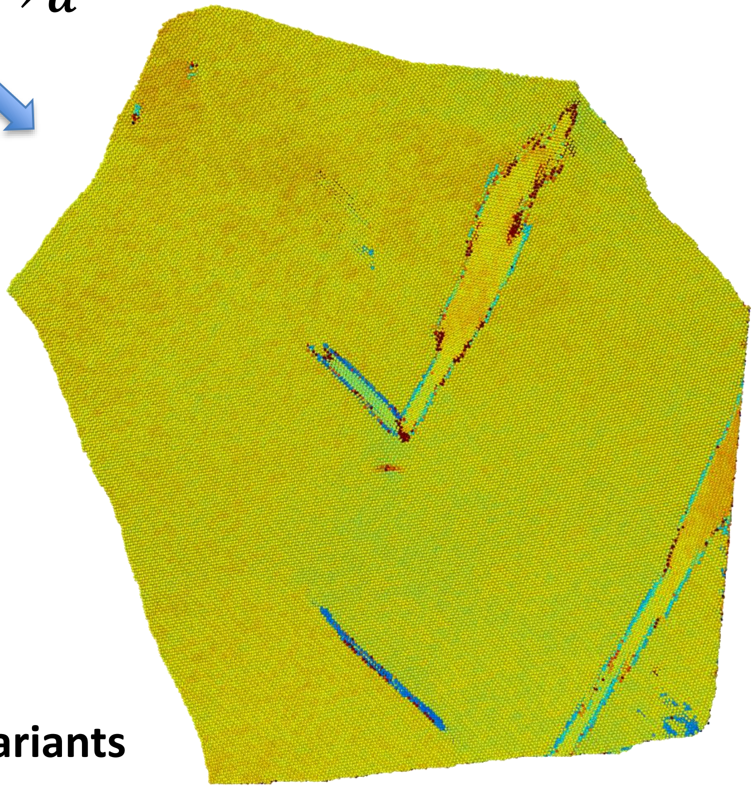
$\alpha \rightarrow \varepsilon$



5 HCP variants

Orientation

$\varepsilon \rightarrow \alpha$



2 Twin variants

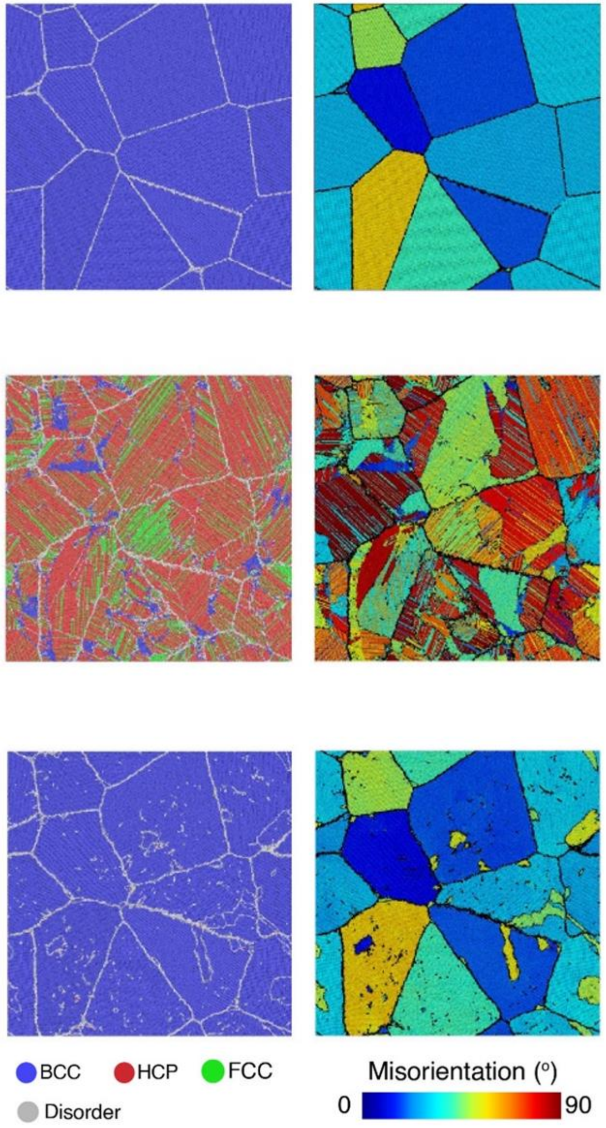
- Reverse $\varepsilon \rightarrow \alpha$ transformation initiates at the boundaries between the hcp variants

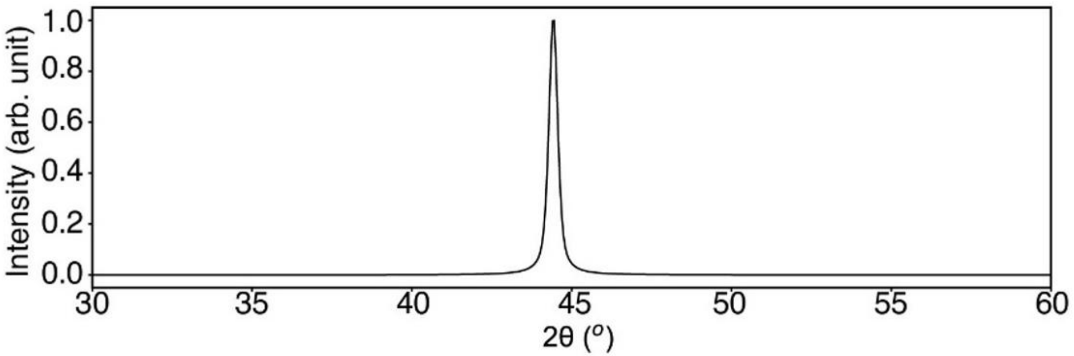
Deformation + Virtual Texture Analysis + Virtual Diffraction

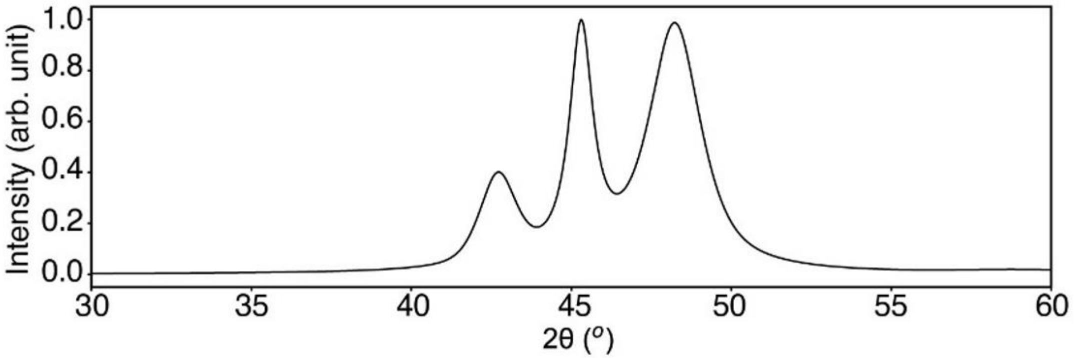
Initial

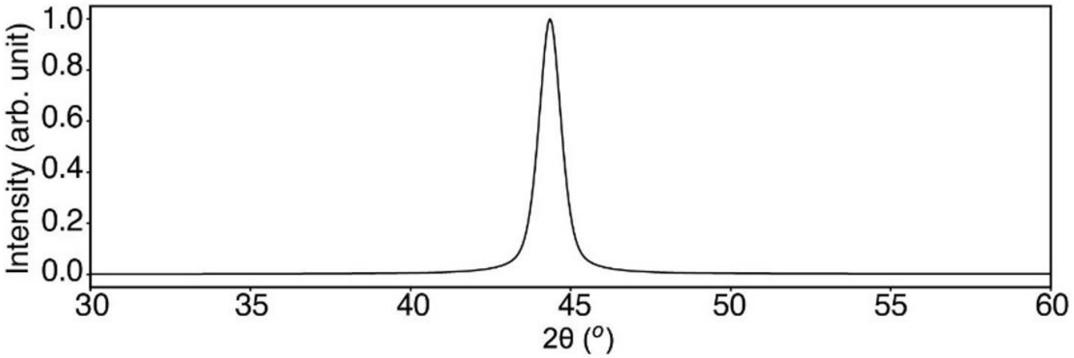
Compressed

Release

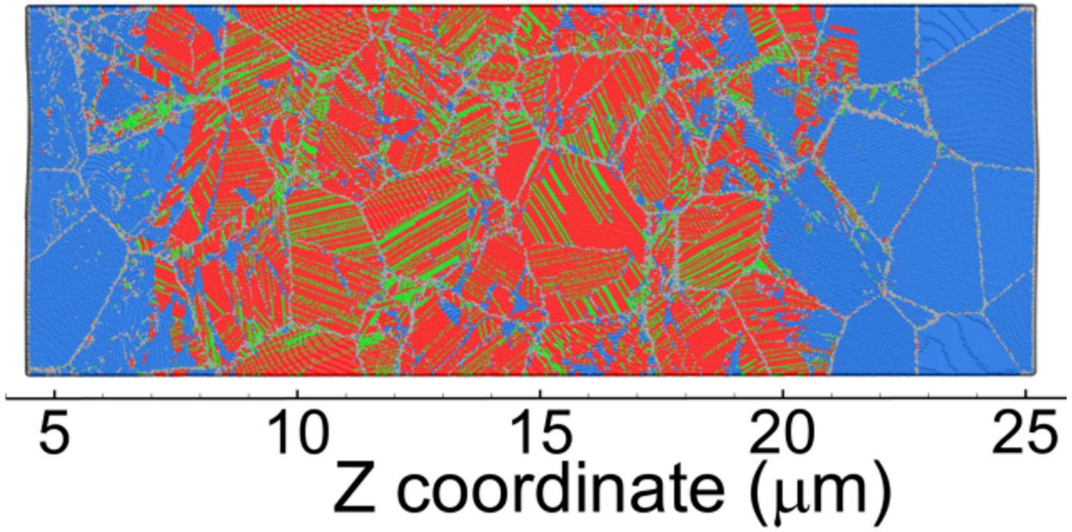


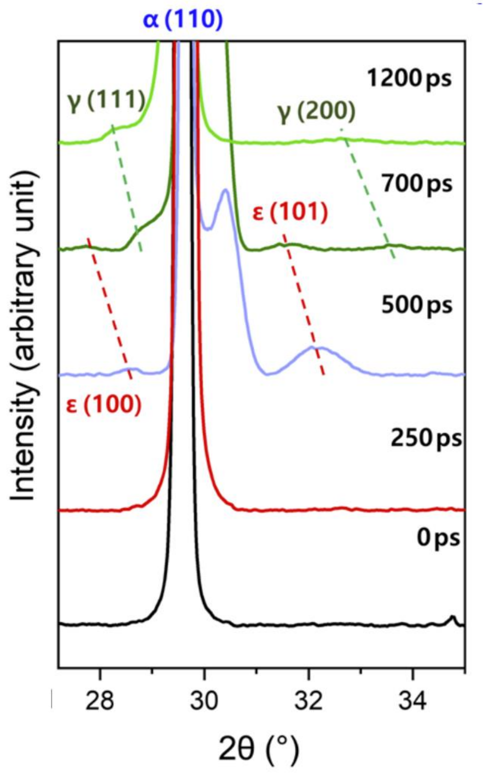




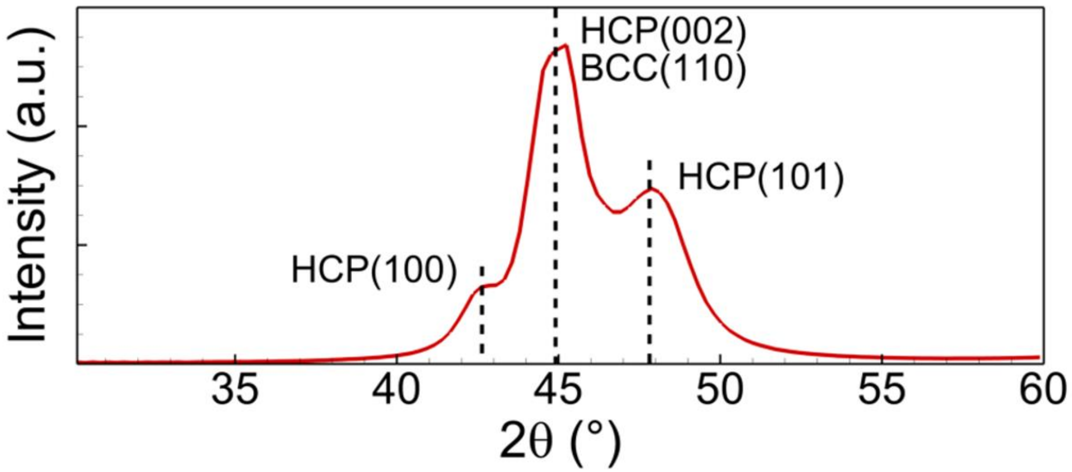


Replicating *in situ* Diffraction Experiments using QCGD





- ■ Microstructure:
  - Uncompressed BCC Fe
  - Phase-transformed HCP Fe
  - Relaxed BCC Fe

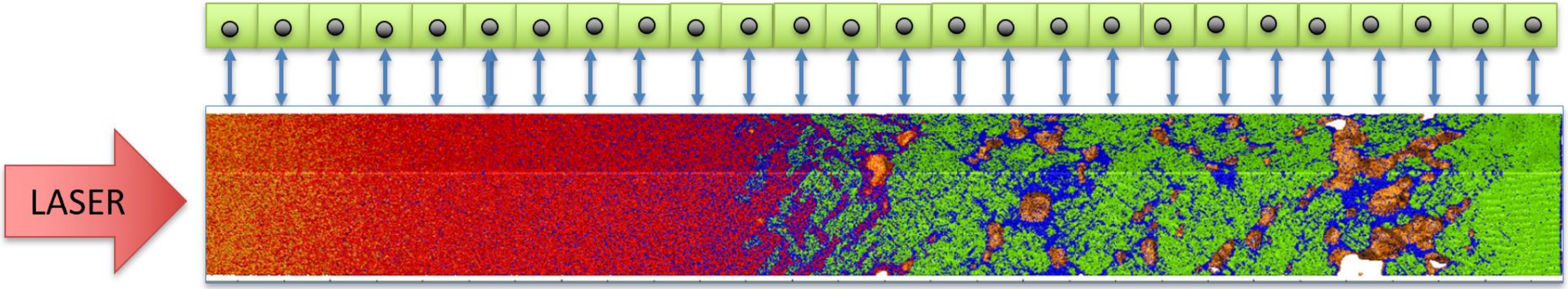


The mesoscale simulations with virtual diffraction allow investigation of mesoscale phenomenon where experimental interpretation is challenging.

Modeling Laser-Metal Interactions: A Hybrid Atomistic-Continuum Method

Electrons

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \frac{\partial}{\partial z}\left(K_e(T_e, T_l)\frac{\partial}{\partial z}T_e\right) - G(T_e - T_l) + S(z, t)$$



Lattice

$$C_l(T_l)\frac{\partial T_l}{\partial t} = G(T_e - T_l)$$

$$T_l^{cell} = \sum_{i=1}^{N^{cell}} m_i\left(\vec{v}_i^{\,T}\right)^2 \Big/ \left(3k_B N^{cell}\right)$$

e: electron

l: lattice

C: heat capacity

K: thermal conductivity

G: electron-phonon coupling factor

S: Source term for laser energy deposition

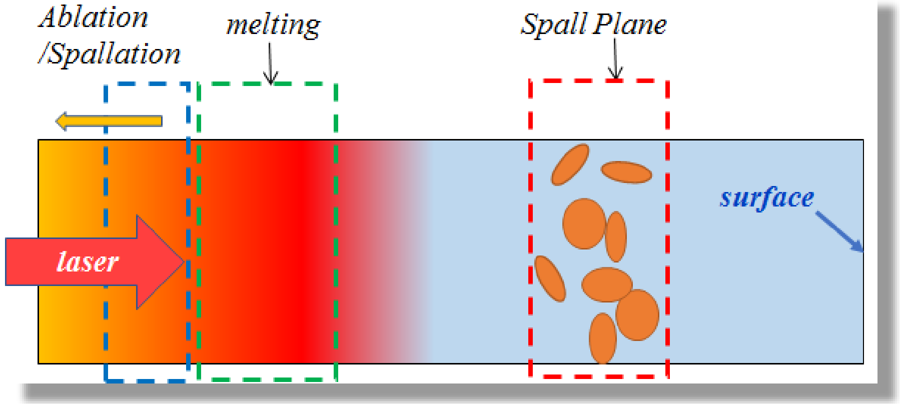
- Continuum TTM describes laser energy absorption/dissipation and electron temperature evolution.
- Classical MD provides the description of lattice superheating and atomic movements during simulation.

Laser Shock Compression and Spall Failure: Al

Experiment al details:

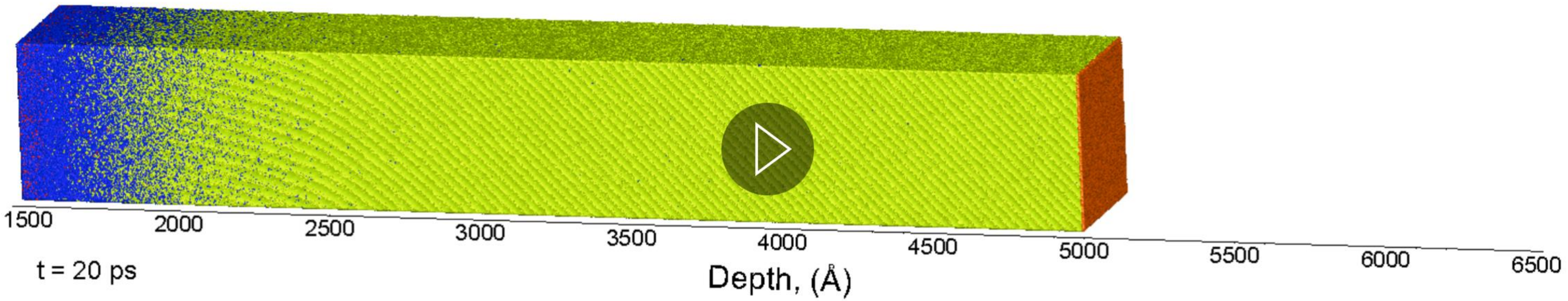
- 500 nm Al foil
- Fluence =13 KJ/m^2
- Laser: τ_L = 150 fs

[S. I. Ashitkov et al. *JETP Letters*. (2010)]



Density Function Theory (DFT): temperature-dependence of

- Electron thermal conductivity (K_e^{solid}, K_e^{liquid})
- Electron-phonon coupling factor (G)
- Electron heat capacity (C_e)



● FCC ● Liquid ● Surface ● HCP ● Disordered ● BCC

[Galitskiy et al., JAP (2018)]

Laser Shock Compression and Spall Failure: Al

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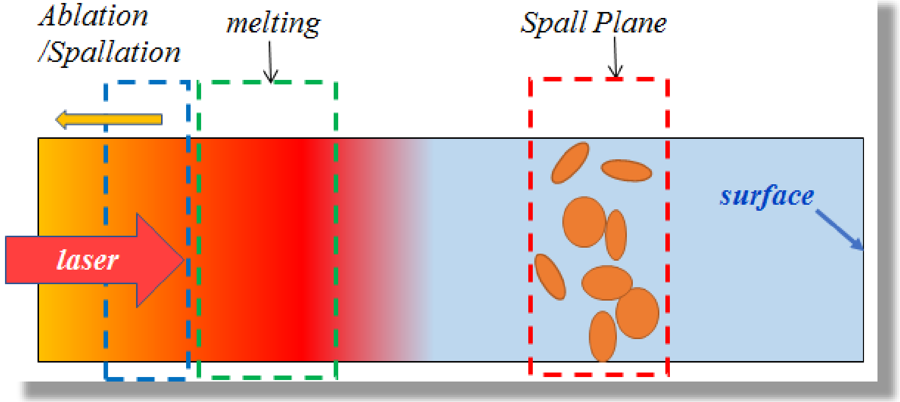
[S. I. Ashitkov et al. *JETP Letters.* (2010)]



Density Function Theory (DFT): temperature-dependence of

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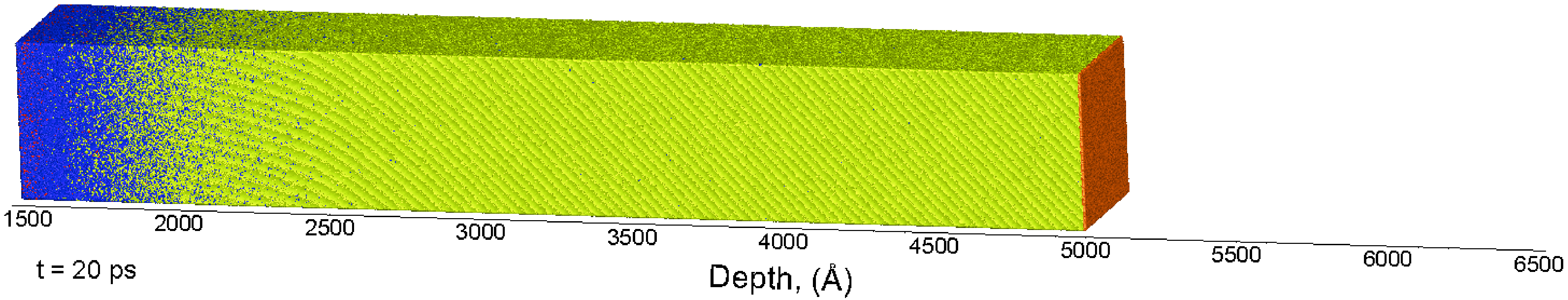


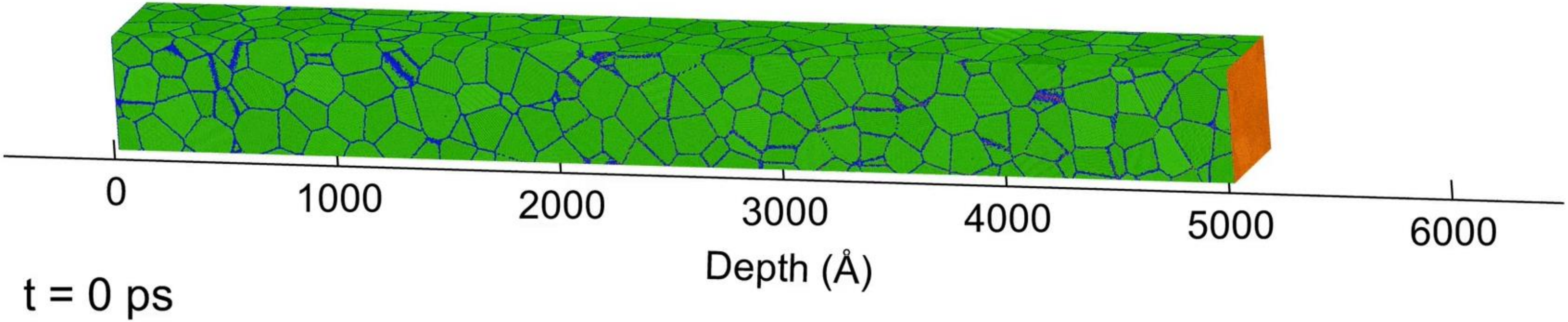
● FCC ● Liquid ● Surface ● HCP ● Disordered ● BCC

[Galitskiy et al., JAP (2018)]

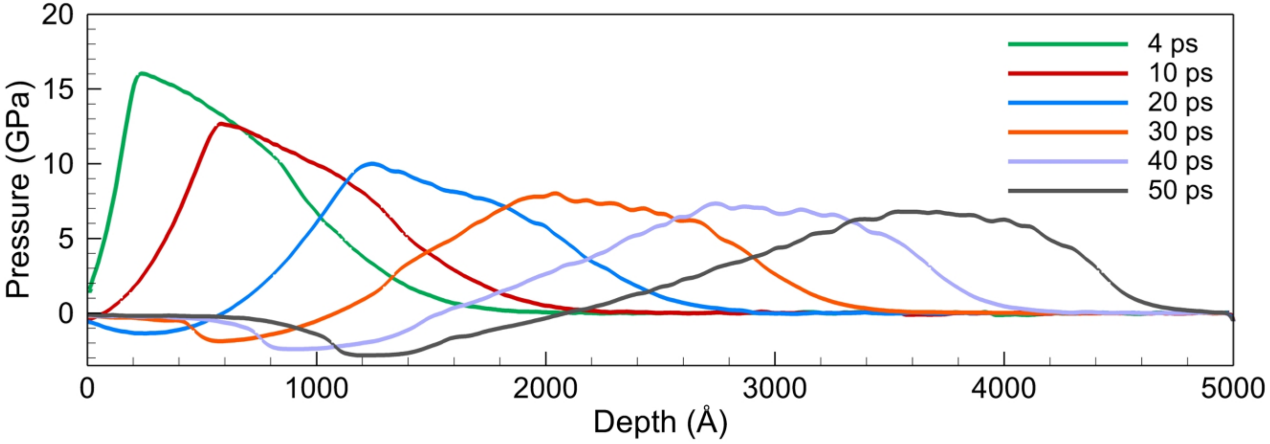
Laser Shock Compression and Spall Failure: Al

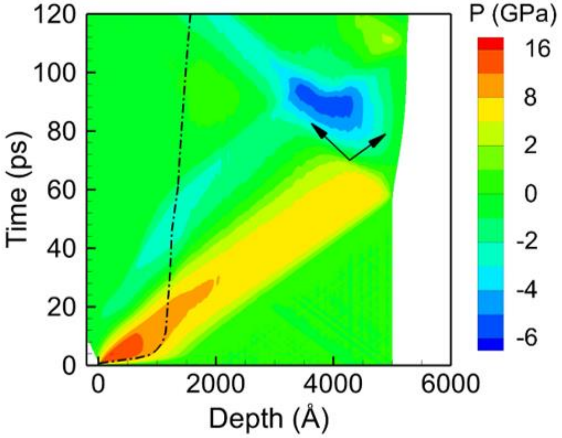
Laser fluence of 13 KJ/m^2 with a pulse duration (τ) of 150 fs.

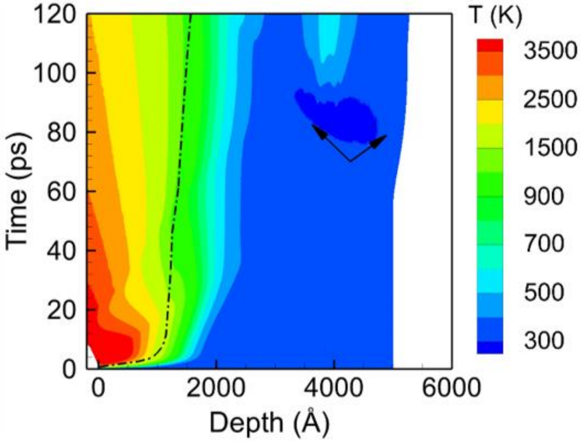
🟢 FCC
🔴 Liquid
🟠 Surface
🟡 HCP
🔵 Disordered
🔵 BCC



σ_{spall} = 5.3 GPa (Exp = 5.7 GPa)





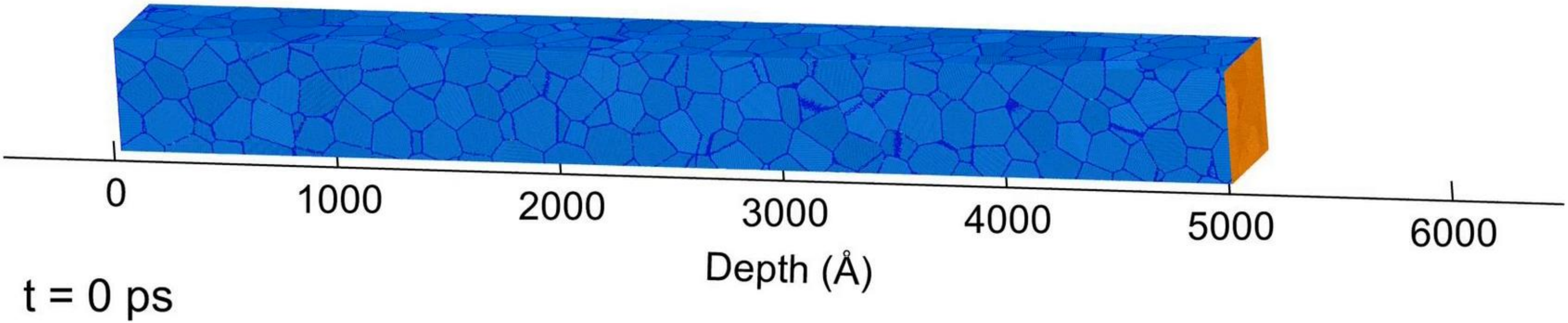


[Chen et al., JAP (in review)]

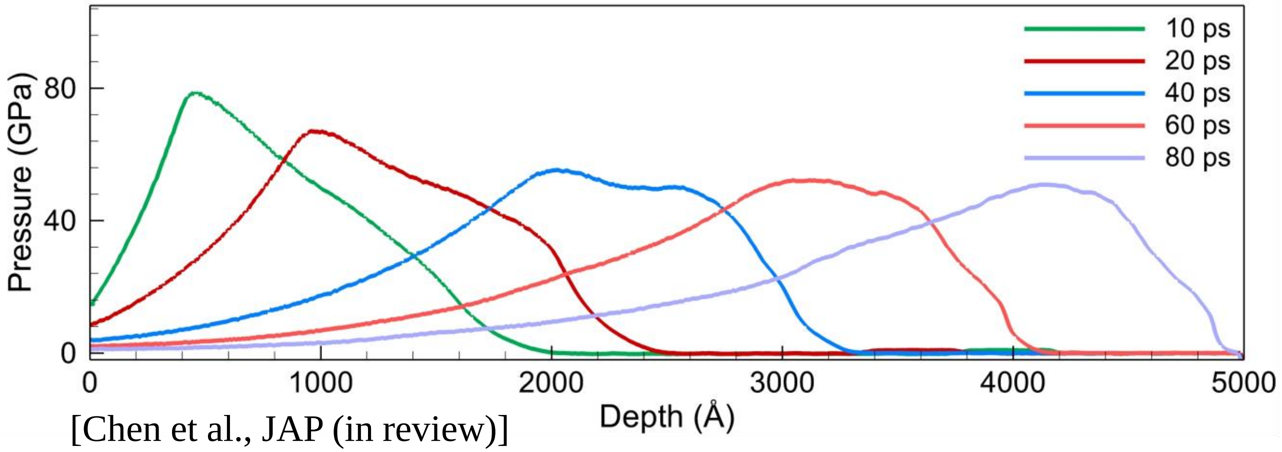
Laser Shock Compression and Spall Failure: Ta

Laser fluence (*F*) of 29 KJ/m^2 and a pulse duration (τ) of 500 fs

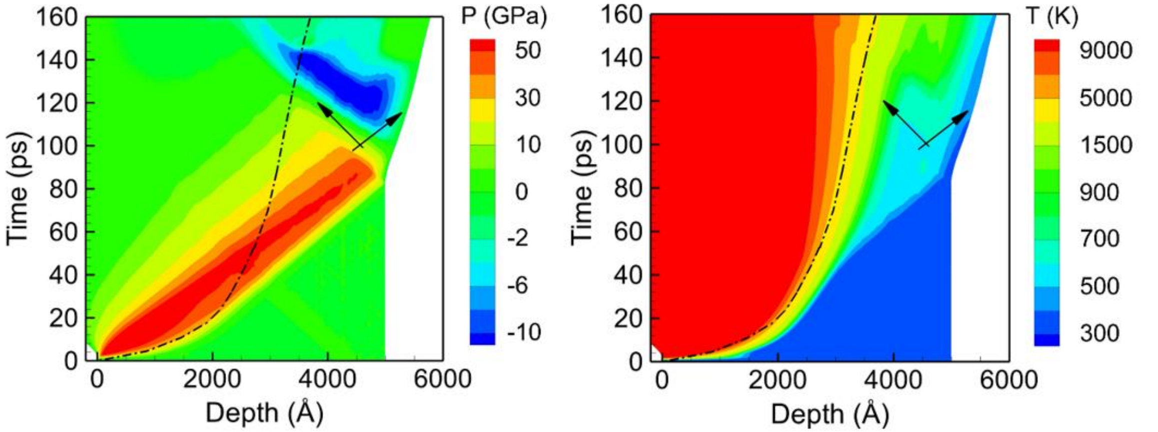
🟢 FCC 🔴 Liquid 🟠 Surface 🟡 HCP 🔵 Disordered 🔵 BCC



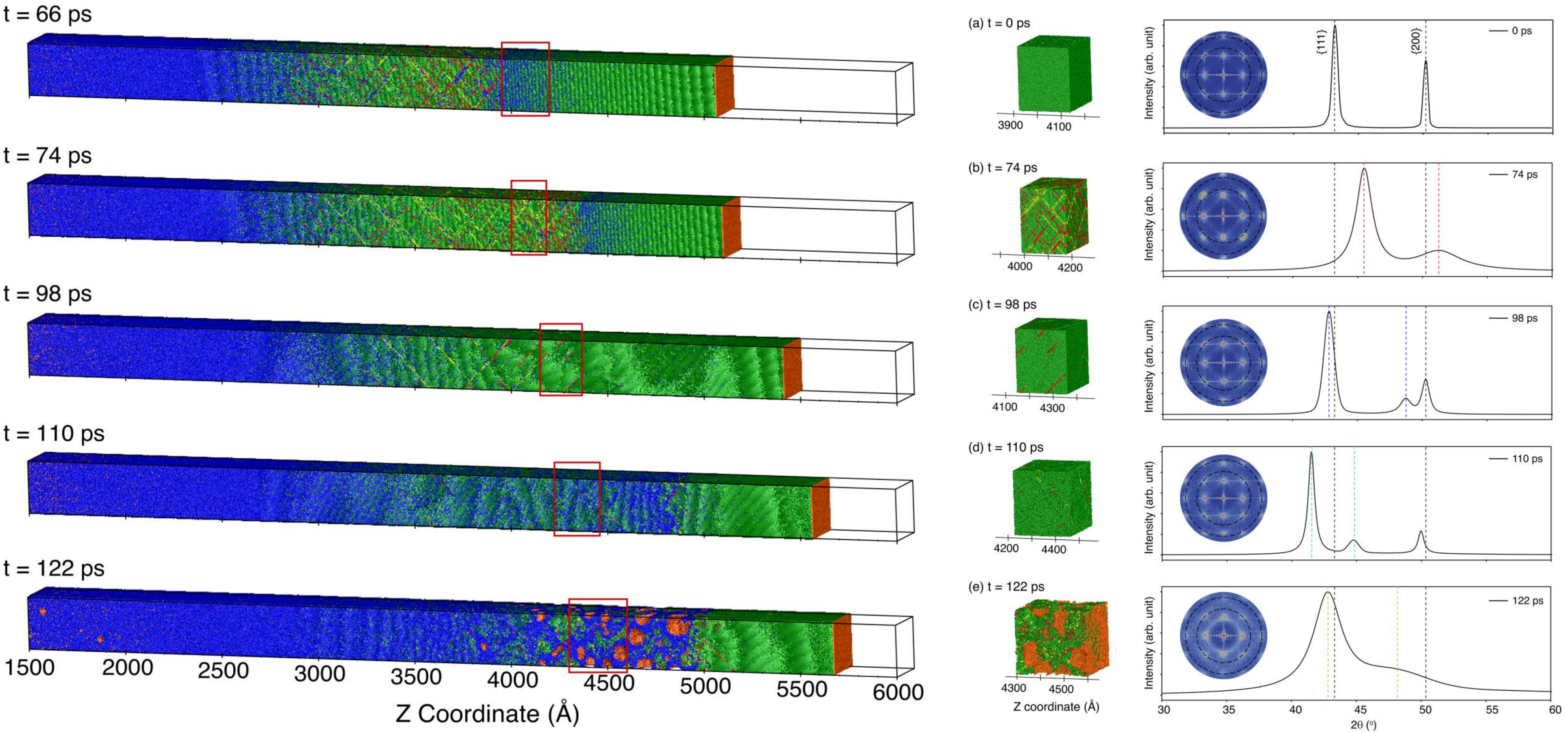
σ_{spall} = 17.7 Gpa (Exp = 26.7 Gpa)



[Chen et al., JAP (in review)]



In Situ Diffraction Laser Shock Compression and Spall Failure: Cu

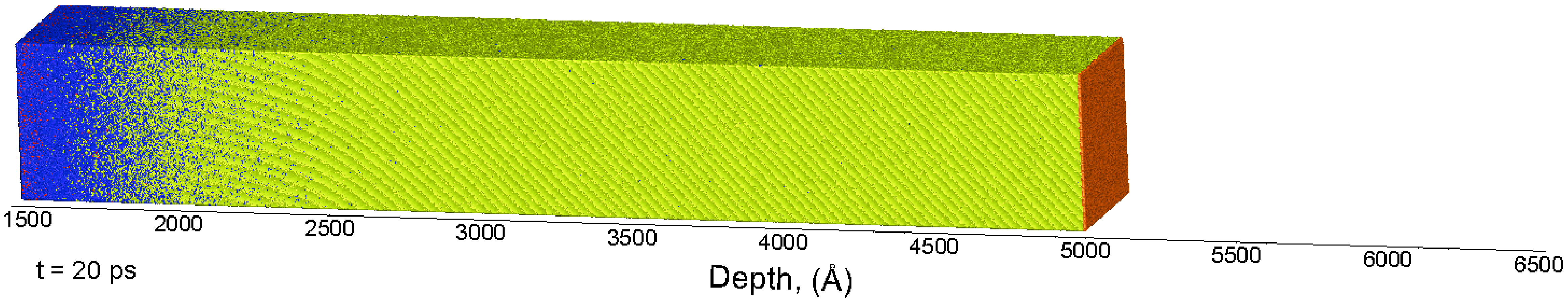


[Echeverria et al., Comp. Mater. Sci (2021)]

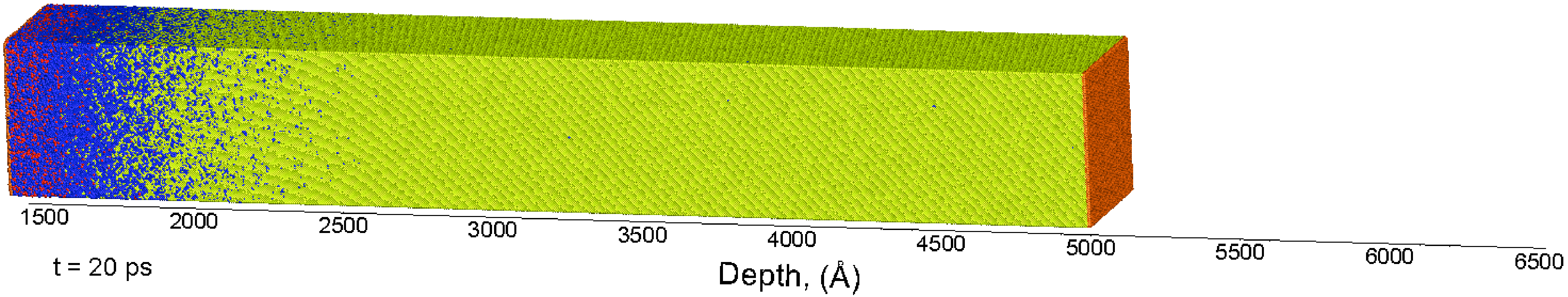
Maser-Metal Interactions at the Mesoscales: QCGD/TTM

Laser Fluence: 13 KJ/m^2; Pulse 150 fs

MD



L2-QCGD



🟥 Liquid 🟧 Surface 🟦 Disordered 🟩 FCC

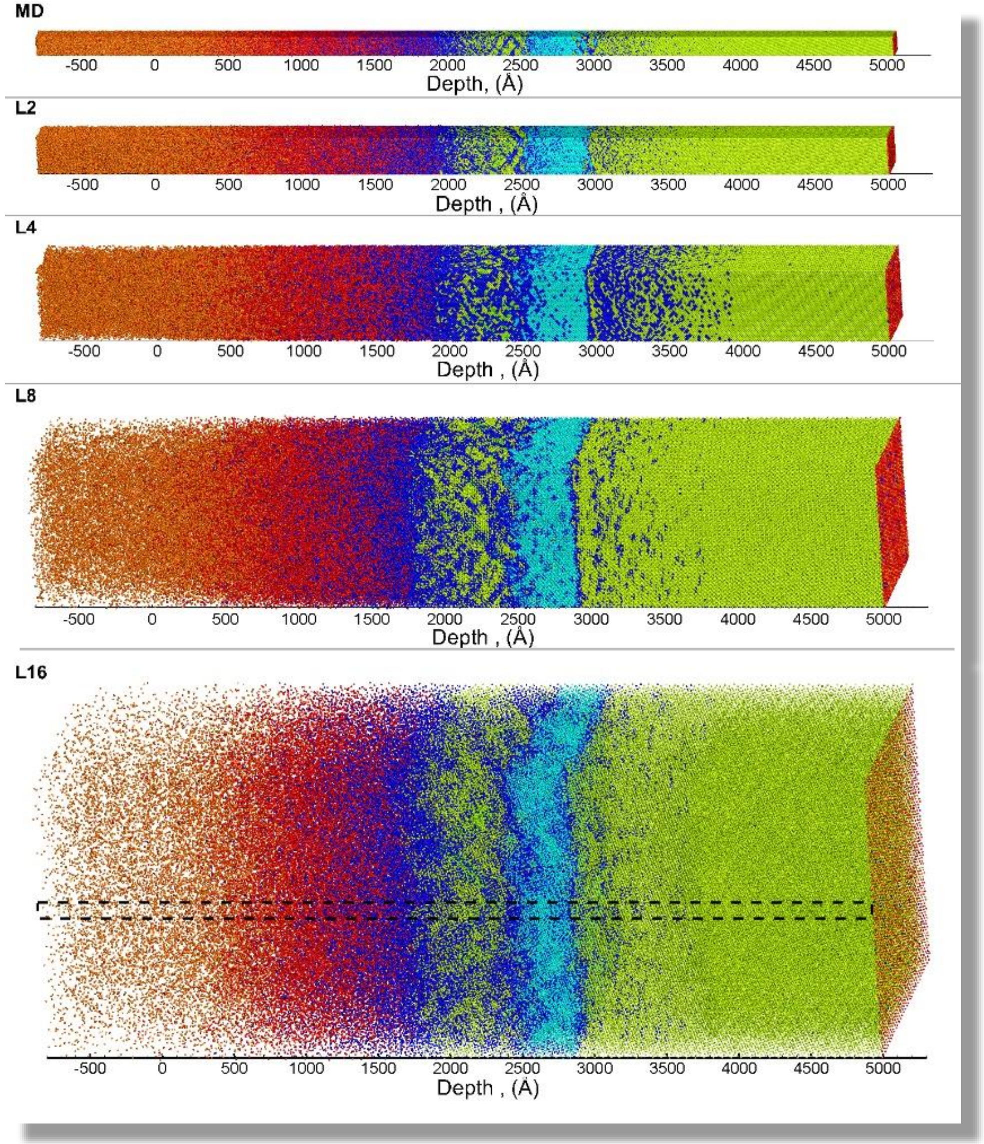
QCGD-TTM Scaling: Higher Levels of Coarsening

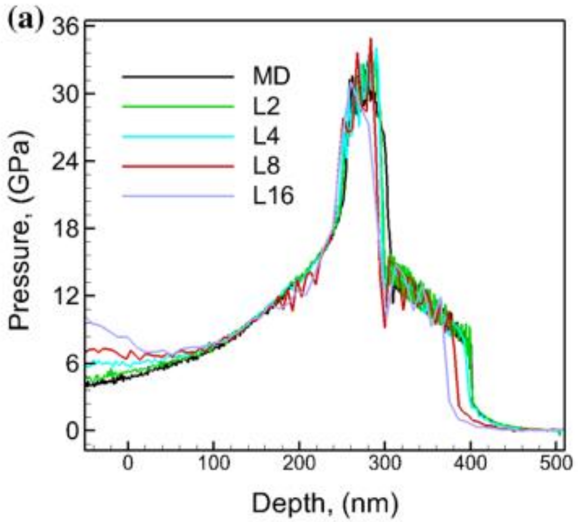
- 500 nm length (Z) Al thin film subjected to high energetic (I ~ 10^{17} W/m^2) ultra-fast laser (τ = 150 fs)
- QCGD level 2-16 compares excellent with MD data

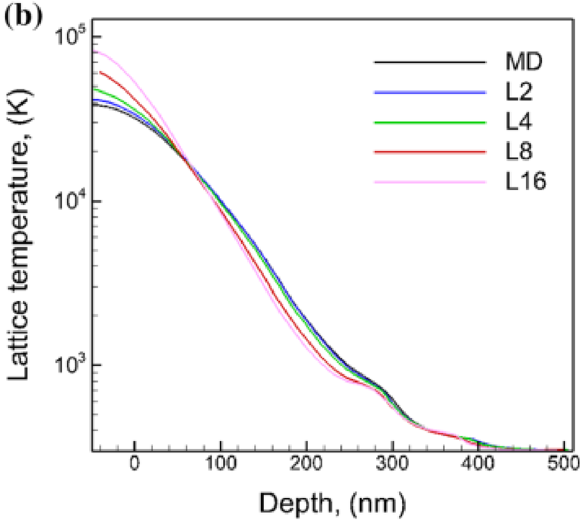
🟧 Gas 🟥 Liquid 🟦 Disordered

🟩 FCC 🟦 BCC

Microstructure evolution (ablation, melting, phase transformation) predicted with higher levels of coarsening in QCGD compares very well MD predicted evolution





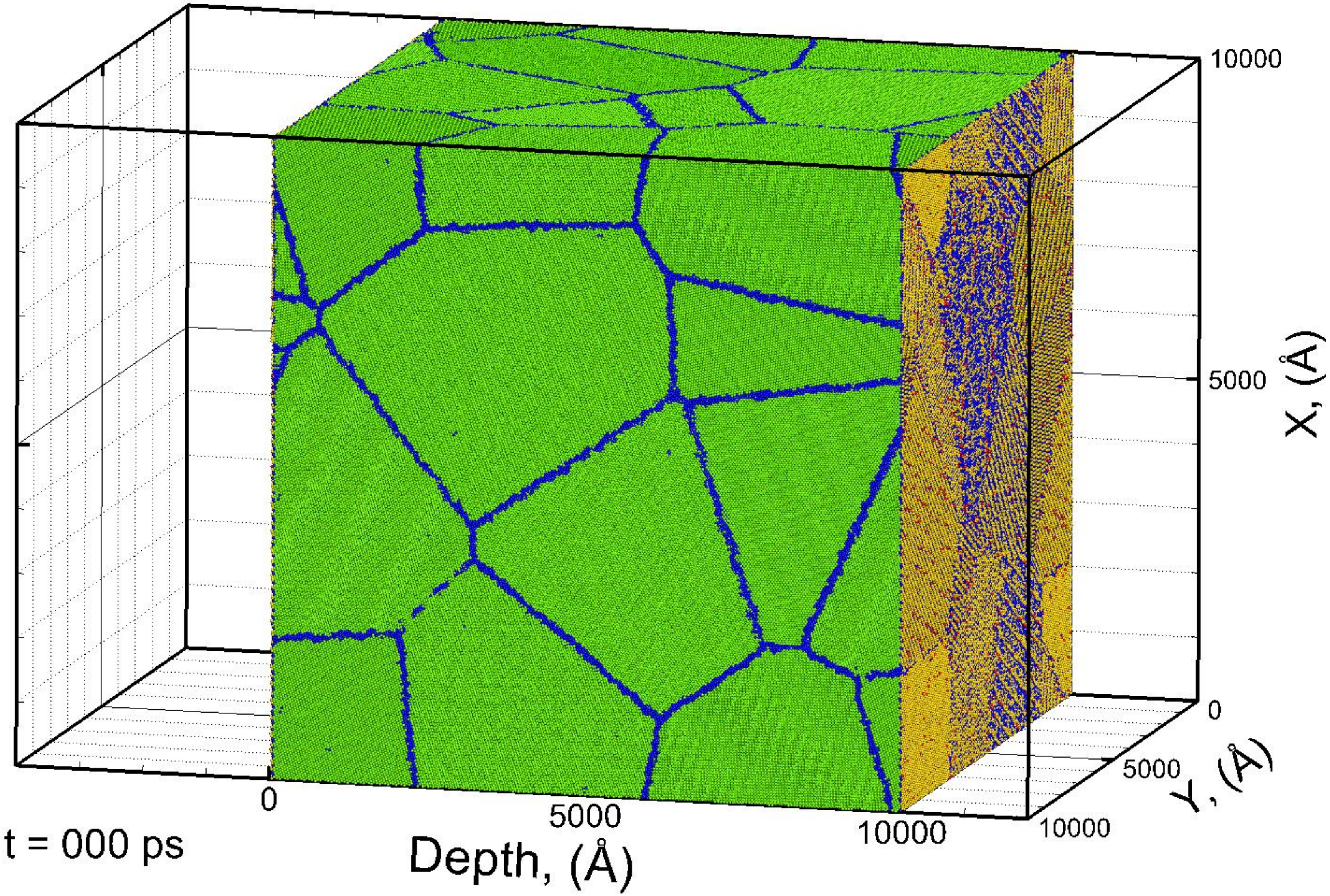


Laser-Shock Loading at Experimental Scales

Laser fluence: 13 KJ/m^2

Pulse duration (τ): 150 fs.

Polycr-Al: d = 500 nm



🟥 Liquid 🟧 Surface 🟦 Disordered 🟩 FCC

Laser-Shock Loading at Experimental Scales

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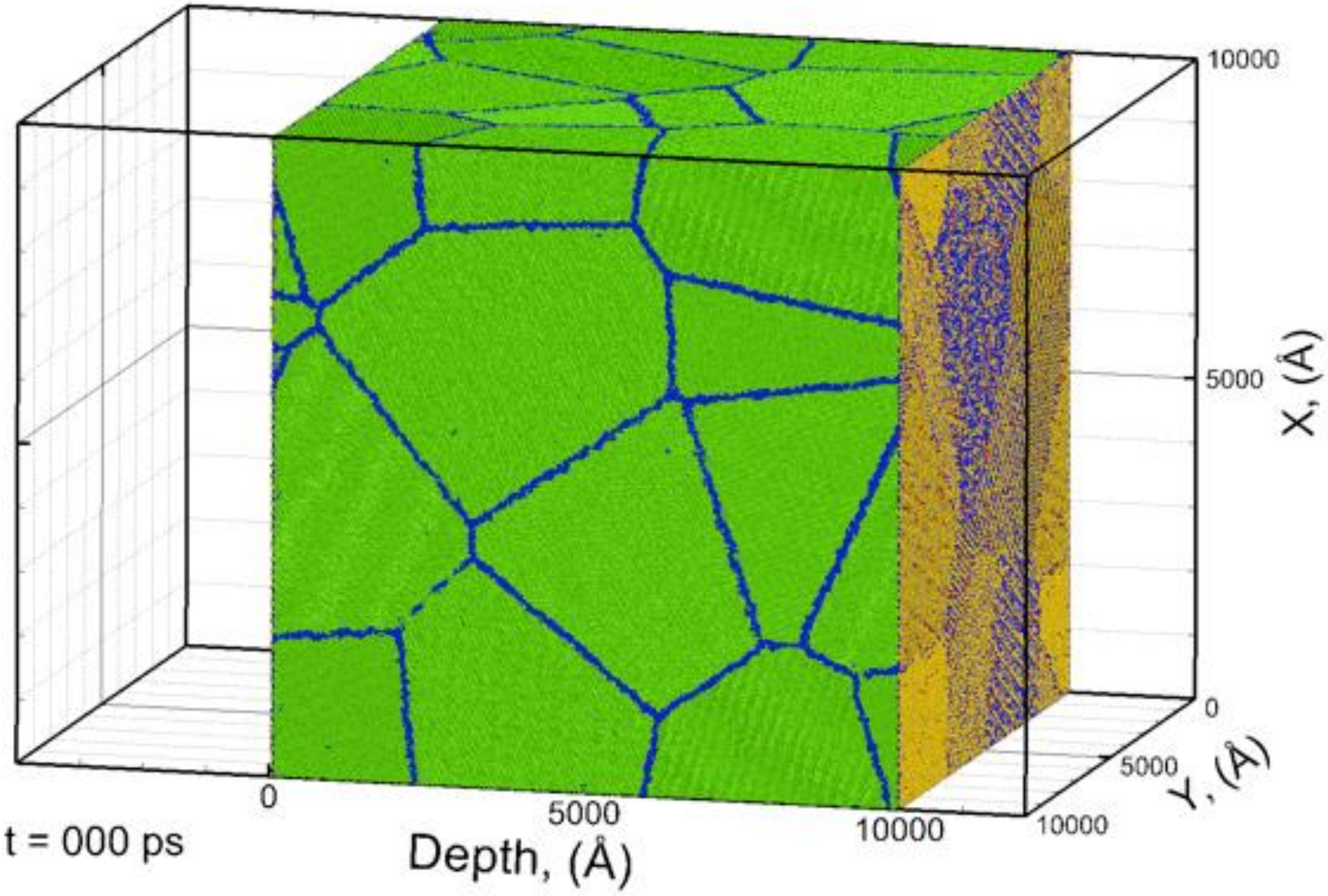

🟥 Liquid 🟧 Surface 🟦 Disordered 🟩 FCC

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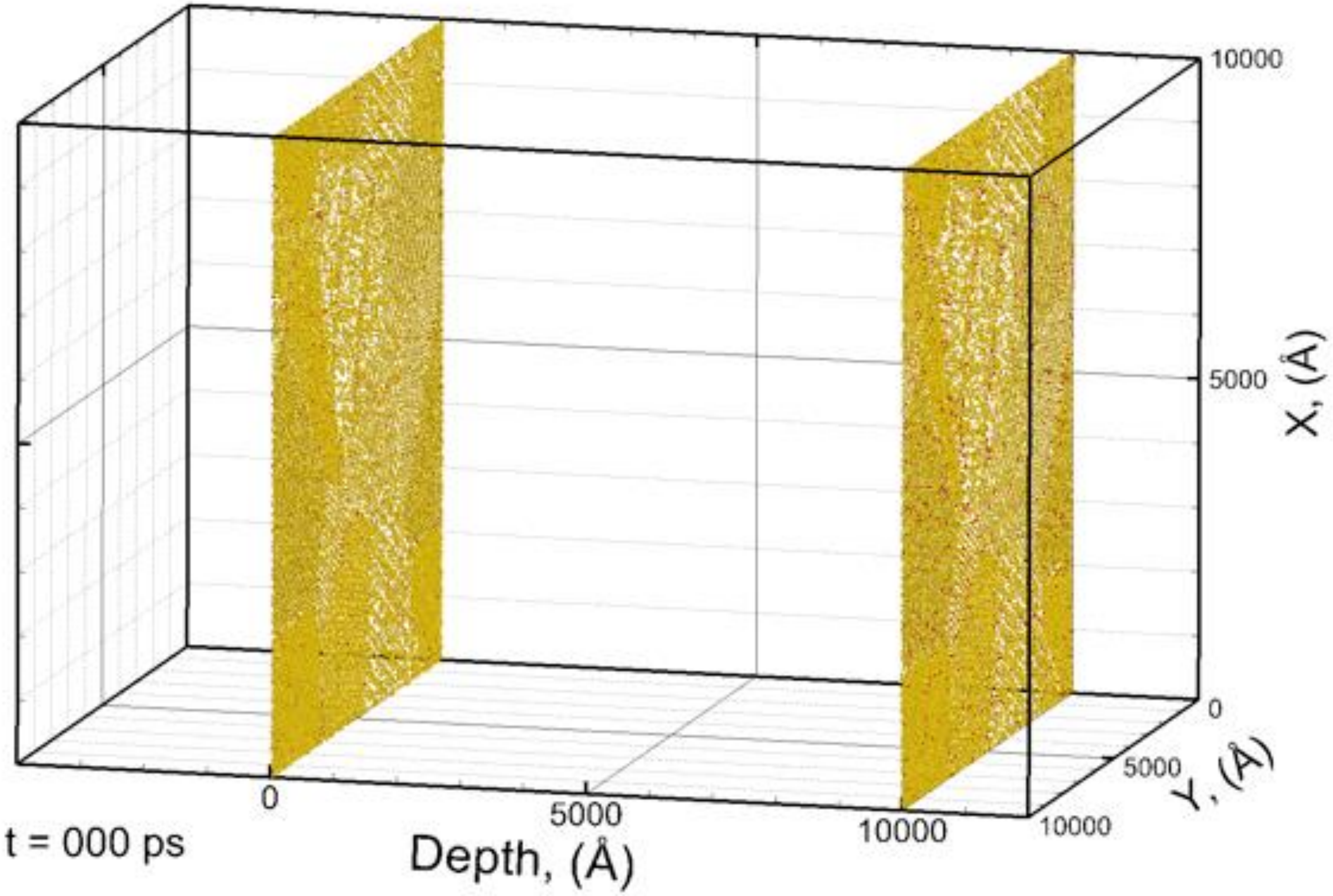
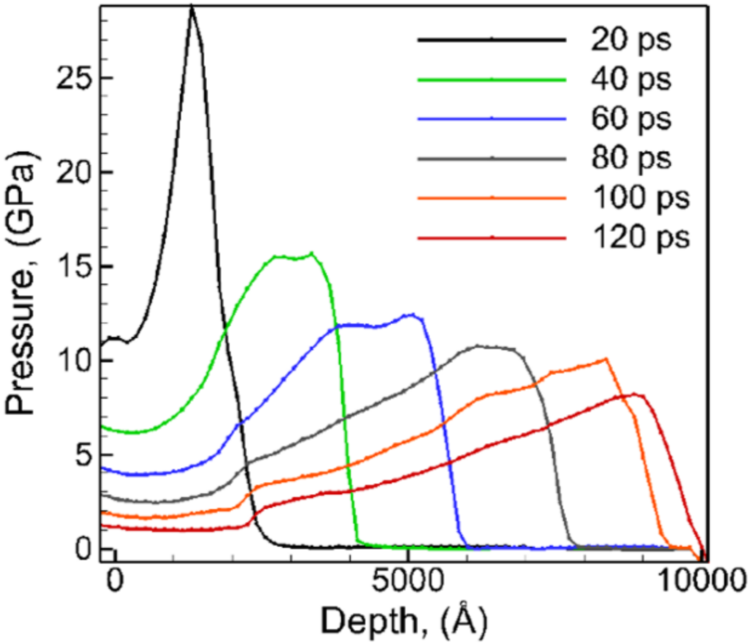
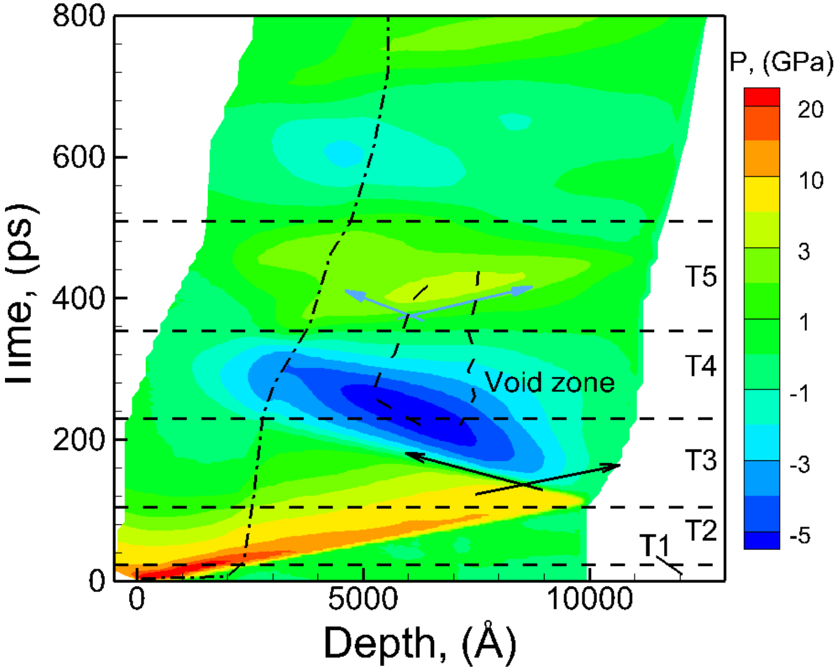
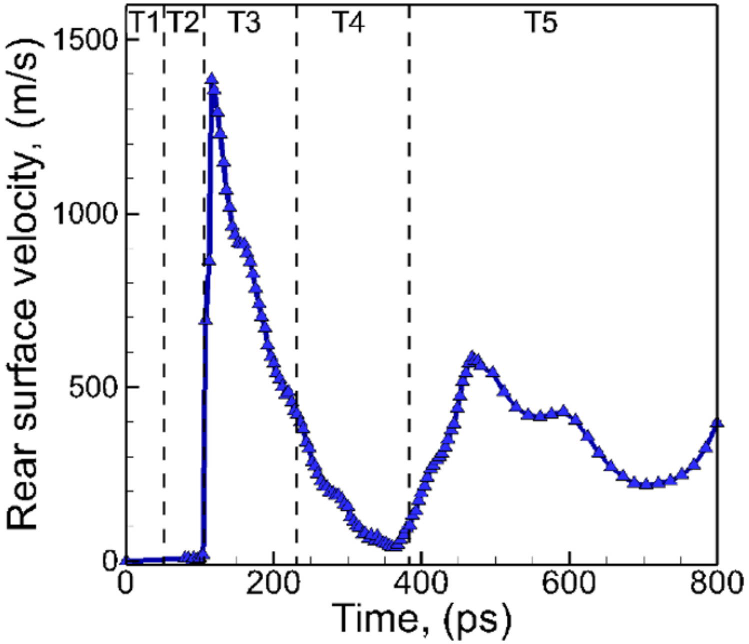


🟥 Liquid 🟧 Surface 🟦 Disordered 🟩 FCC

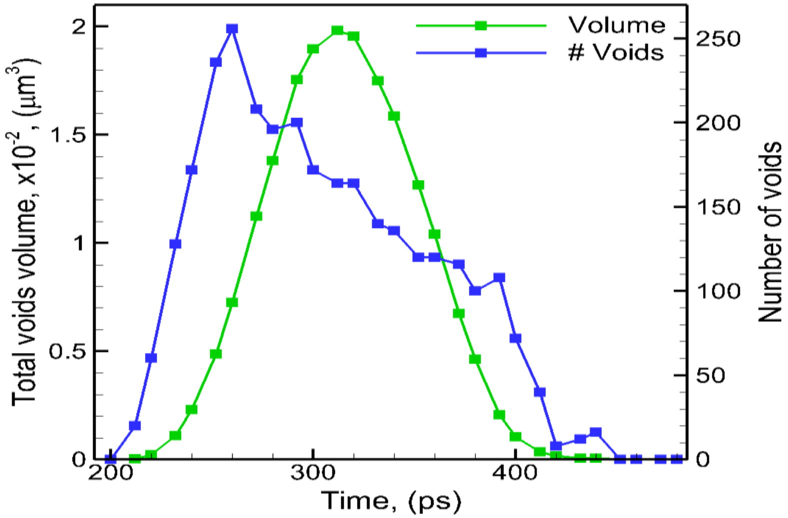
Laser-Shock Loading at Experimental Scales







- Nucleation of voids at 200 ps, their growth and coalescence till 320 ps
- The tensile wave reflects from the solid-liquid interface to create a recompression wave
- Gradual decrease of void number and void volume up to zero
- Recompression signal is observed in rear surface velocity profiles



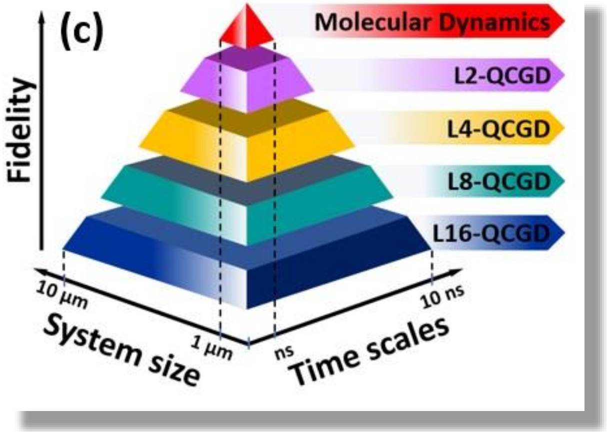
Summary

- MD simulations using virtual diffraction enable the characterization of plasticity contributions during shock compression in polycrystalline BCC microstructures (Ta and Fe)

- A new virtual texture (VirTex) analysis approach to characterize phase transformation and twinning variants in deformed microstructures generated using MD simulations.

- A hybrid atomistic-continuum method (MD-TTM) enables the modeling of laser material interactions providing an accurate description of ablation, melting, and shock phenomena at the atomic scales

- **Quasi-coarse-grained dynamics** is a **low-fidelity model that** enables the scaling of MD simulations to the mesoscales and retains the MD-predicted plasticity contributions from dislocation slip, phase transformation, and twinning in metals and **allows *in situ* diffraction at experimental scales**



[Mishra et al., *J. mater. Sci.* (2022)]

- **Current focus:** Building digital twins of laser shock experiments to build a database of virtual diffractograms

Acknowledgements

- **Funding**

  This material is based upon work supported by the Department of Energy, National Nuclear Security Administration under Award No. DE-NA0003857. Any opinions, findings, and conclusions or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the National Nuclear Security Administration.

  CREDDS
  Center for Research Excellence
  on Dynamically Deformed Solids

  NNSA
  National Nuclear Security Administration

- **Computing Resources:**

  ⟶ High Performance Computing (HPC) facilities at UCONN

- **Collaborations:**

  ⟶ Saryu Fensin (LANL), Remi Dingreville (SNL), Mukul Kumar (LLNL), John Lind (LLNL), KT Ramesh (JHU)

- **Contact:** dongare@uconn.edu

Thank you