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Phase Field Modeling and Simulation of Deformation and Failure

S&T Campaign: Sciences for Lethality & Protection
Tier 2 Subtopic: Dynamic Failure of Materials

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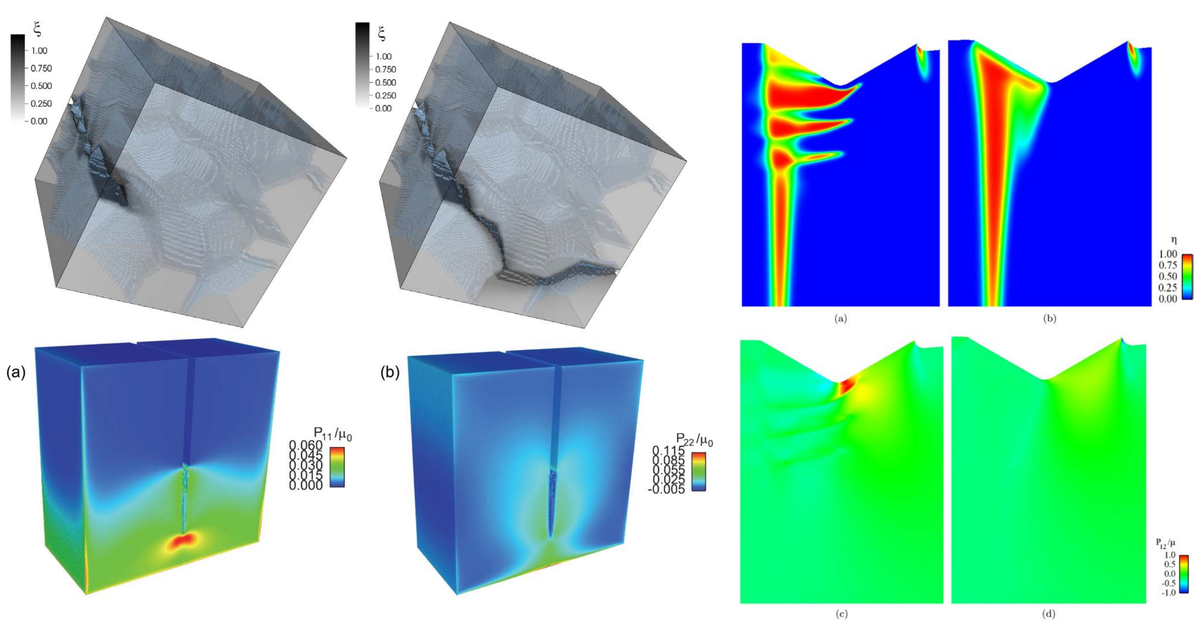
Research Objectives

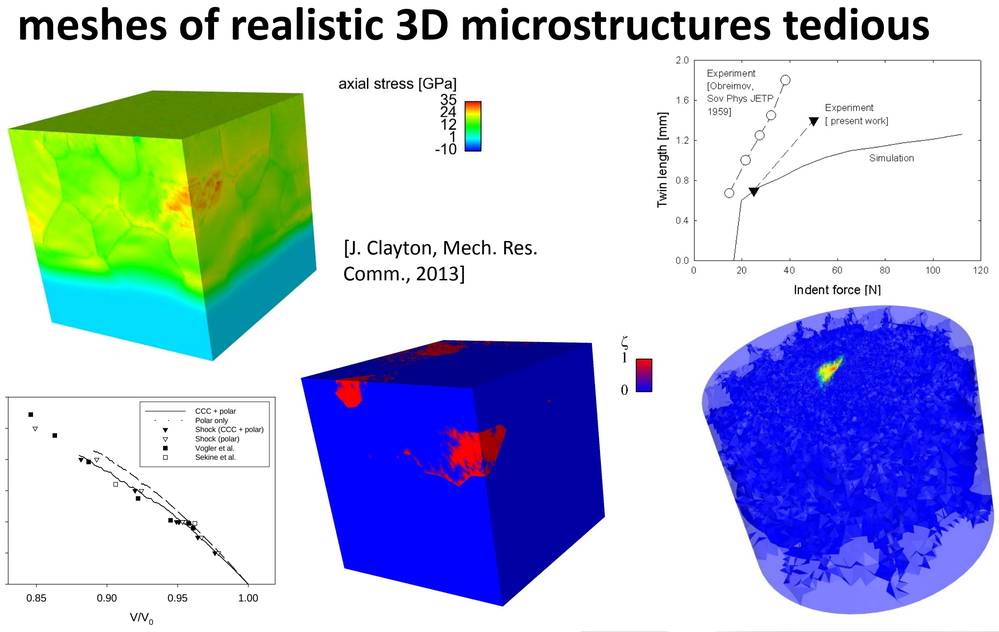
- Understand and predict most important deformation mechanisms in crystalline solids used in Protection and Lethality systems (armor and munitions)
- Inform higher length-scale models used in system design
- Approach accounts for nonlinearities and coupling among mechanisms with minimal model parameters

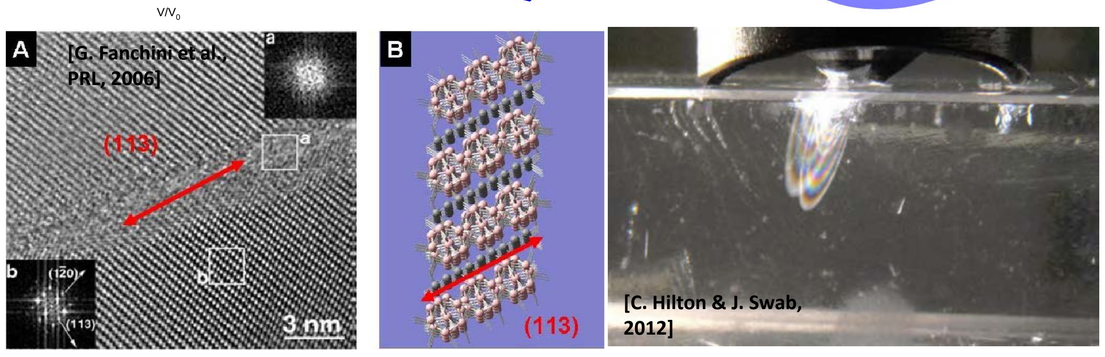


Phase field simulations of fracture (left [4,5]) and twinning (right [2])

Challenges

- Numerical resolution: mechanisms at competing length and time scales (e.g., thin interfaces in large specimens)
- Complexity: numerous potential planes and directions for twinning, slip, localization, cleavage fracture, etc.
- Generation of statistically representative finite element meshes of realistic 3D microstructures tedious





Amorphization (left) and twinning (right): simulations and experiments

ARL Facilities and Capabilities Available to Support Collaborative Research

- Specialized modeling/simulation tools: modular C++ code with XDMF I/O, scalable parallelization [J. Knap, ARL-CISD]
- Parallel ARL DSRC computing facilities
- Significant results to date
  - First nonlinear phase field theory for twinning, validation for twin nucleation in Mg [1]
  - Simulation of indentation-induced twinning in calcite and sapphire [2]
  - Correct prediction of twin nucleation or crack extension in calcite, sapphire, and Mg [3]
  - First phase field theory of fracture with elastic nonlinearity and cleavage anisotropy, with validation and analysis of inclusions [4]
  - Prediction of Hall-Petch scaling of strength and ductility, effects of anisotropy and GB phases on fracture for SiC and Zn polycrystals [5]
  - First nonlinear phase field theory for coupled twinning and fracture, with new analytical solutions and criteria for stability and failure [6]
  - First phase field model of stress-induced localization; predicts trends in boron carbide [7]
- ARL expertise in computer science [8] and theoretical continuum mechanics of anisotropic solids [9]
- References

[1] J. Clayton, J. Knap (2011) Physica D 240, 841-858.
[2] J. Clayton, J. Knap (2011) Mod. Sim. Mater. Sci. Eng. 19, 085005.
[3] J. Clayton, J. Knap (2013) Acta Mater. 61, 5341-5353.
[4] J. Clayton, J. Knap (2014) Int. J. Fracture 189, 139-148.
[5] J. Clayton, J. Knap (2015) Comp. Mater. Sci., in press.
[6] J. Clayton, J. Knap (2015) Philos. Mag., in review.
[7] J. Clayton (2014) AIMS Mater. Sci. 1, 143-158.
[8] J. Knap, J. Clayton (2011) ARL-MR-760.
[9] J. Clayton (2011) Nonlinear Mechanics of Crystals, Springer, Dordrecht.

Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- Characterization and validation experiments: energy pathways for inelastic deformation mechanisms; quantitative study of sequential or concurrent twinning, slip, fracture, and structural transformations at mesoscale
- Specialized laboratory facilities: Advanced Photon Source, in-situ and post-mortem microstructure characterization
- Expertise in efficient microstructure rendering & meshing
- Suggestions for innovative new research approaches to address stated research objectives: multi-scale modeling

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