Scalable Algorithms for Simulating Dislocations in Micro-structured Crystals

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S&T Campaign: Computational Sciences
Predictive Simulation Sciences

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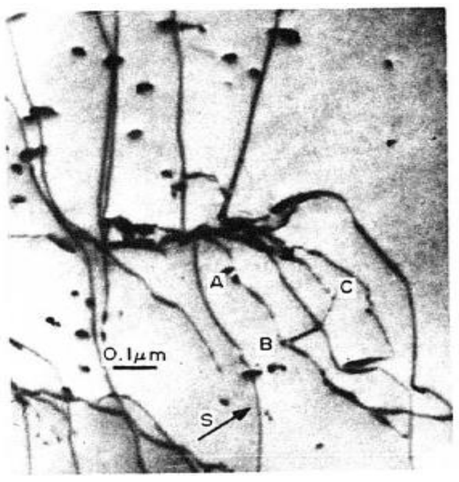
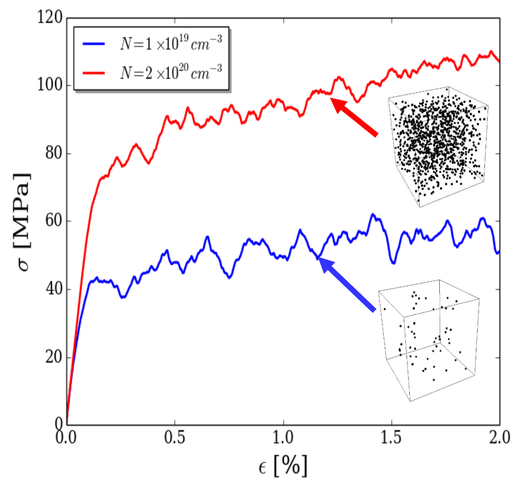
Research Objective

- Develop algorithms to explore the interactions of dislocations with microstructure in materials
- Manipulate material properties through creative control of dislocation mechanisms



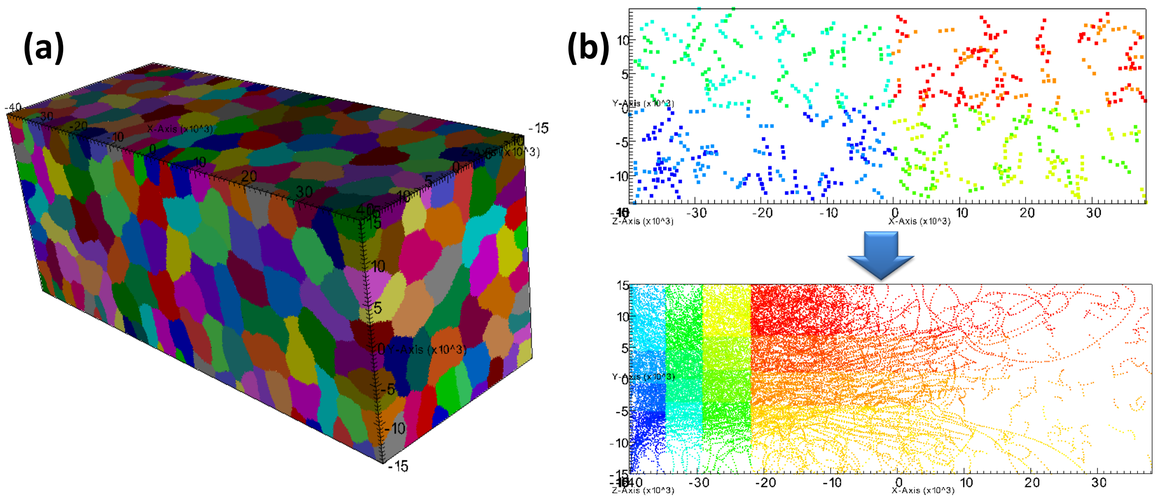
Experimentally observed hardening due to the pinning of dislocations at voids (Manusmare and Leighly, Jr. 1976).



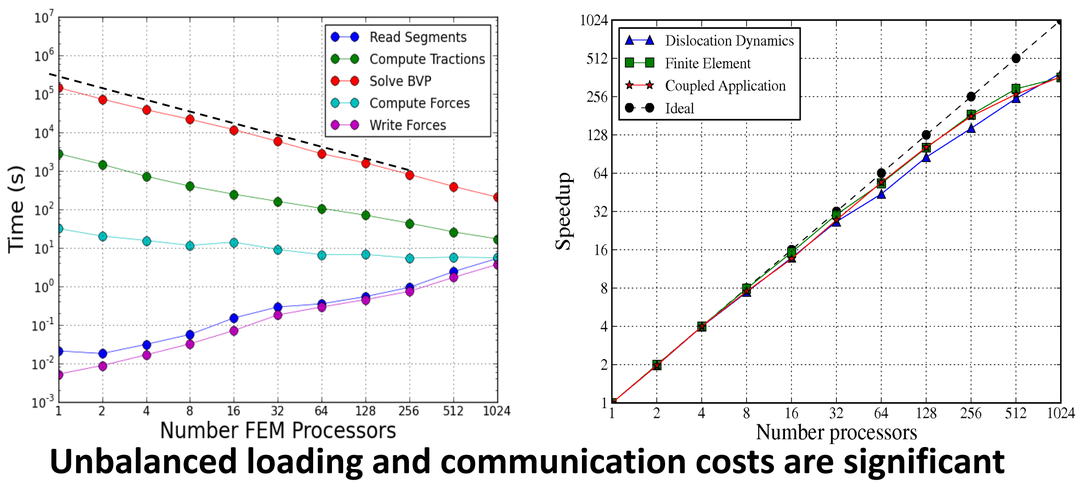
Simulated stress-strain curves demonstrating the increased hardening due to increasing void density.

Challenges

- Limited understanding of dislocation behavior near microstructure
- Large computational expense required to accurately capture the effects of microstructure on dislocations



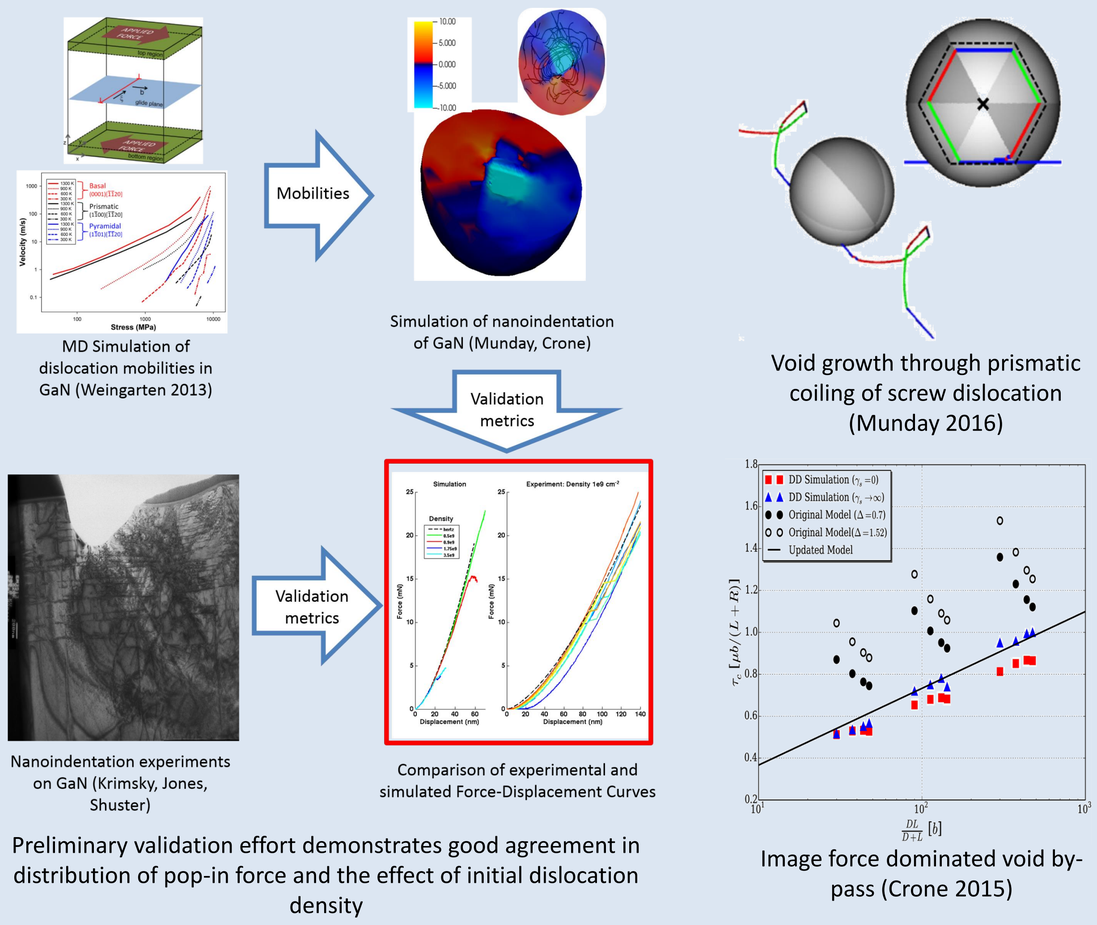
Independent static (a) and dynamic (b) domain decompositions present challenges in load balancing and code-coupling.



Unbalanced loading and communication costs are significant obstacles to large-scale parallel efficiency.

ARL Facilities and Capabilities Available to Support Collaborative Research

- DoD supercomputing resource center (DSRC)
- Expertise in multiscale and code-coupling frameworks
- Initial algorithm demonstrated 100x increase in tractable system sizes from previous state-of-the-art
- Preliminary validation shows good qualitative agreement with experimentally observed dislocation-microsturcture interactions



MD Simulation of dislocation mobilities in GaN (Weingarten 2013)

Simulation of nanoindentation of GaN (Munday, Crone)

Void growth through prismatic coiling of screw dislocation (Munday 2016)

Nanoindentation experiments on GaN (Krimsky, Jones, Shuster)

Comparison of experimental and simulated Force-Displacement Curves

Image force dominated void by-pass (Crone 2015)

Preliminary validation effort demonstrates good agreement in distribution of pop-in force and the effect of initial dislocation density

- **Recent publications:**
  - L.B. Munday, J.C. Crone and J. Knap, *Acta Mat.* 103, 217 (2015).
  - J.C. Crone, L.B. Munday and J. Knap, *Acta Mat.* 101, 40 (2015).
  - L.B. Munday, J.C. Crone, and J. Knap, Scripta Mat. 103, 65 (2015).
  - J.C. Crone, et al., *MSMSE*. 22, 035014 (2014)
  - K.W. Leiter, J.C. Crone, and J. Knap, J. Comp. Sci., 4, 401 (2013).

Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- Quantum and atomistic simulations to characterize:
  - Dislocation mobility laws for novel Army material
  - Mobility laws for dislocations interacting with surfaces, interfaces and grains
  - Dislocation core and surface energy
- Experimental validation of dislocation models:
  - Dynamic TEM
  - Stress-strain response of single- and poly-crystals with microstructure
  - Nanoindentation

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