Scalable Algorithms for Simulating Dislocations in Micro-structured Crystals

S&T Campaign: Computational Sciences
Predictive Simulation Sciences

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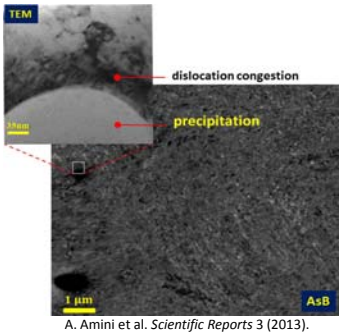
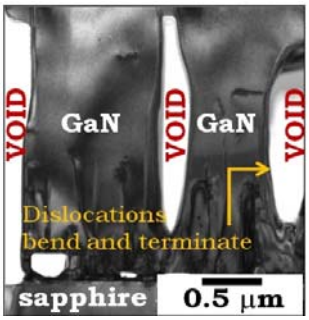
Research Objective

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



A. Amini et al. *Scientific Reports* 3 (2013).



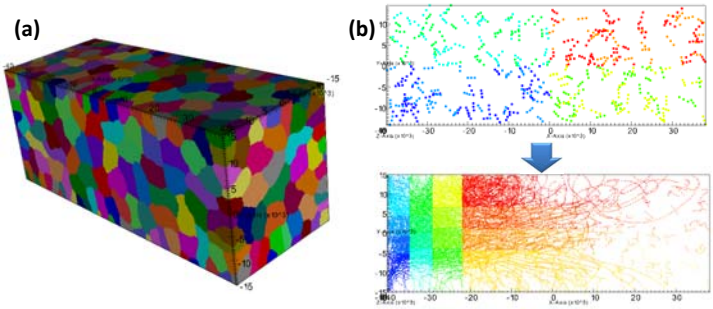
P. Frajtag et al., Appl. Phys. Lett., **98** (2011).

Dislocation interactions with precipitates (a) and voids (b) show significant effect to microstructure, leading to increased dislocation density in (a) and decreased density in (b).

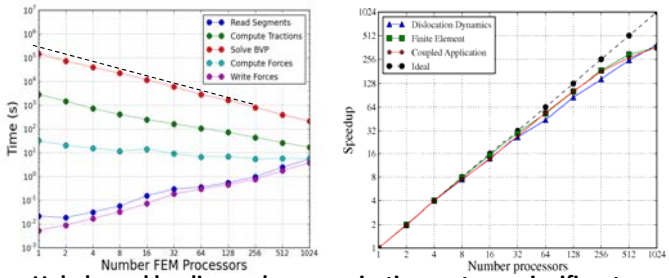
Challenges

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

(a) (b)



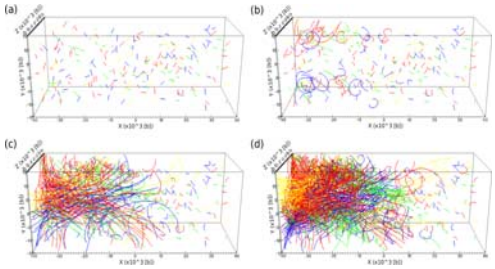
Independent static (a) and dynamic (b) domain decompositions present challenges in load balancing and code-coupling.



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

ARL Facilities and Capabilities Available to Support Collaborative Research

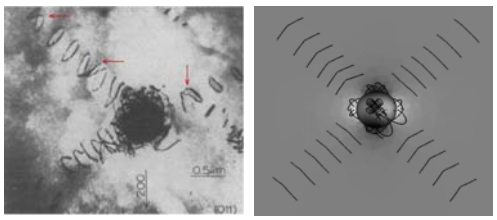
- DoD supercomputing resource center (DSRC) with over 400K compute cores across 10 HPC systems
- Expertise in multiscale and code-coupling frameworks
- Initial algorithm demonstrated 100x increase in tractable system sizes from previous state-of-the-art



Dislocation pile-up due to bending of a cantilever beam represented by over 22M finite element degrees of freedom.

- Preliminary validation shows good qualitative agreement with experimentally observed dislocation-microsturcture interactions

(a) (b)



Dislocation nucleation from an inclusion observed experimentally (a) and through our dislocation dynamics simulator (b).

B Makenas and H. Birnbaum, Acta Metall. 28 (1980)

- Recent publications:
  - J.C. Crone, et al., Modelling Simul. Mater. Sci. Eng. 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

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