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Title: Living in a Material World

Author(s): Hunter, Abigail

Intended for: Seminar at University of Utah as the recipient of the 2020 Alum Award from the Dept. of Mechanical Engineering

Issued: 2020-11-25

Living in a Material World

Abigail Hunter

December 4, 2020

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

LA-UR-20-#####

Thank You!

Regional Academic Collaborations (ReACt)

- **Workshop Goals:**
  - Promote gender balance in the field of computational mechanics and sciences.
  - Provide an opportunity for university researchers to form research collaborations in partnerships with LANL and LLNL.
  - Build relationships between DOE national laboratories and regional universities for academic placements and future workforce.

JANUARY 26-29, 2021

Outline

- **Down the yellow brick road**
  - An overview of my career path
  - Recent career highlights
- **Interesting research (and some about mentoring)**
  - Refractory Multiple Principle Element Alloys (MPEAs)
  - Failure in (Quasi-)Brittle Metals
  - Predicting the Composition of Asteroid 16 Psyche

…and I am a Material Girl

wikipedia.org mypetchicken.com

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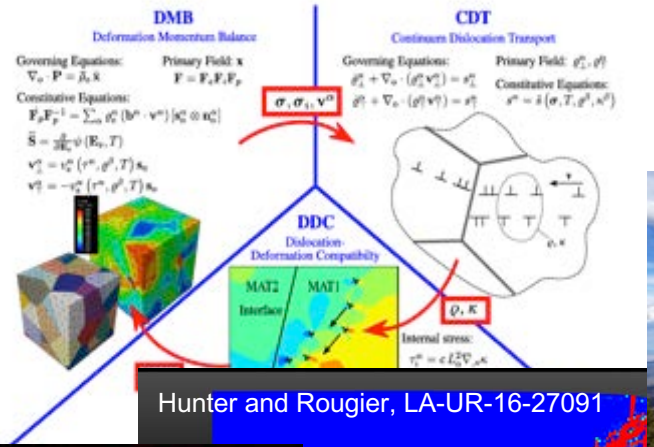
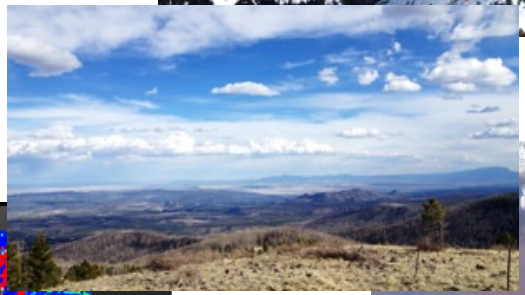
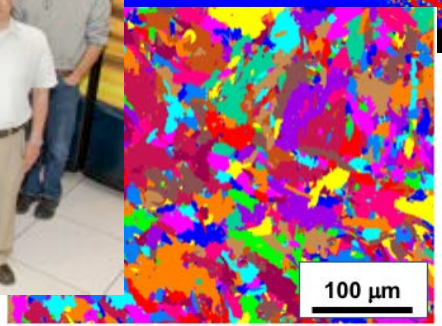
Los Alamos National Laboratory (and New Mexico)

Courtesy of John Carpenter



Hunter and Rougier, LA-UR-16-27091





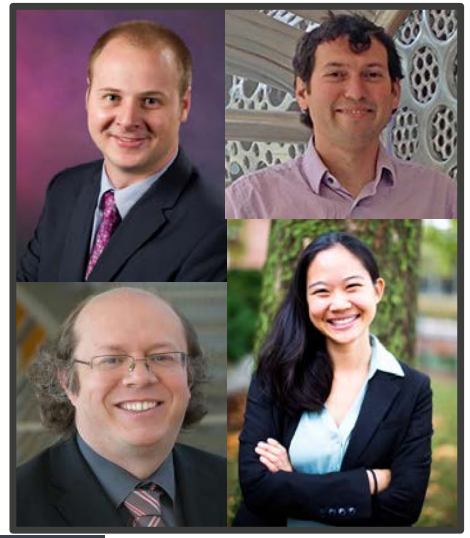
Courtesy of Saryu Fensin

The PECASE award

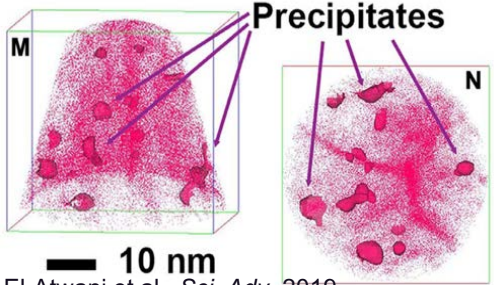
- **"For developing and implementing a *new brittle mechanics model* and *modeling dislocation dynamics*, two capabilities designed to address questions concerning advanced manufacturing of new materials for the stockpile stewardship program; and for *outreach of future STEM professionals.*"**
- **I was nominated in 2016 for the 2015 award cycle.**

Institute for Materials Science (IMS)

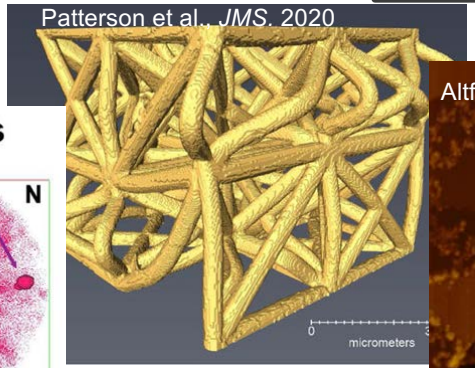
- **Incubate – Innovate – Integrate**
  - Interdisciplinary research and educational center focused on cultivating the advancement of materials science at Los Alamos National Laboratory.
  - Support new, cutting edge research through rapid response grants, new capabilities, etc.
  - Hosting, support and sponsor a range of speakers, seminars, colloquia, research, educational opportunities, workshops, conferences and collaborations

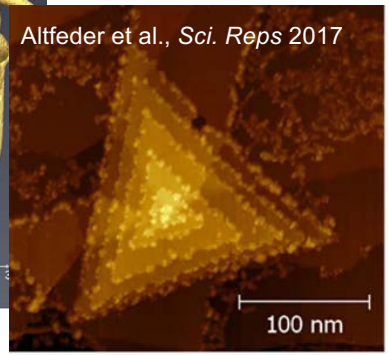


IMS
Institute for Materials Science
Los Alamos



El-Atwani et al., *Sci. Adv.* 2019

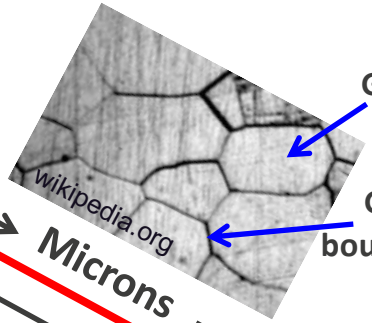




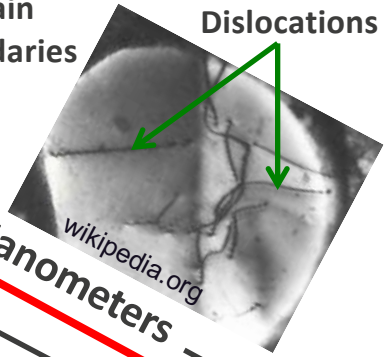
Why and how do we design stronger and lighter materials?

Macroscale/Continuum

Meters



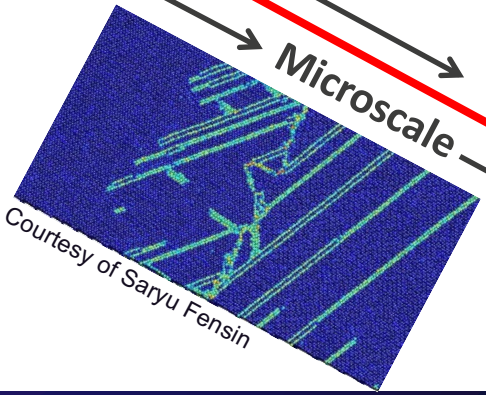
Microns



Nanometers

Mesoscale

Microscale



How do metals deform?

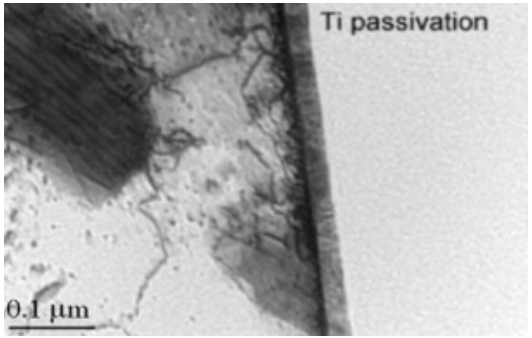
What are metals made of?

What happens in between?

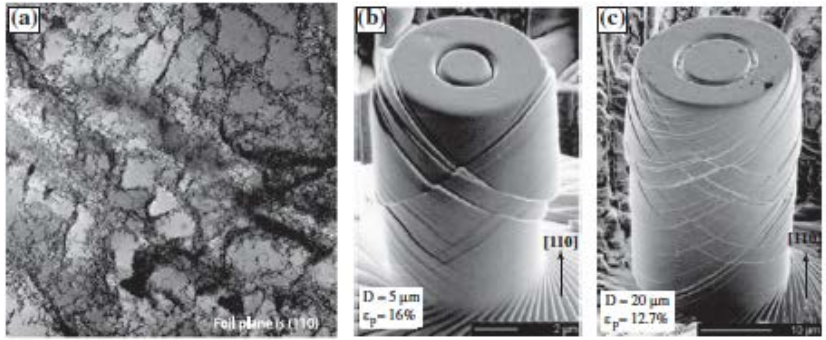
How do we understand and predict material strength?

Dislocations

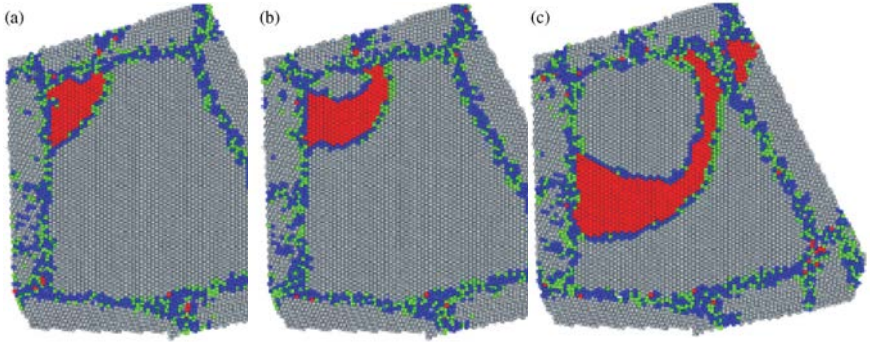
Christian, *Met. Trans. A*, **14A** (1983).



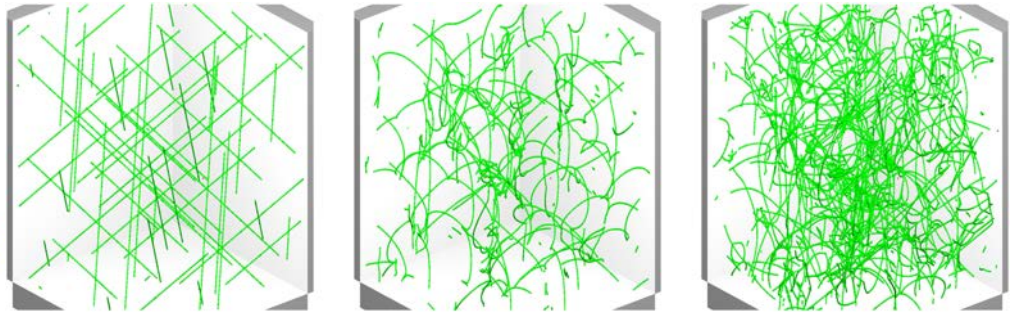
Nicola et al., J. Mech. Phys. Solids, **54** (2006).



El-Awady et al., *Scripta Mat.*, **68** (2013).

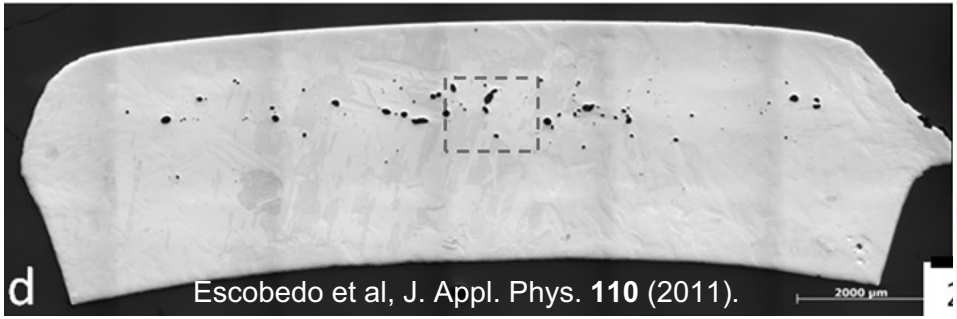


Van Swygenhoven, MSE-A **483-484** (2008).

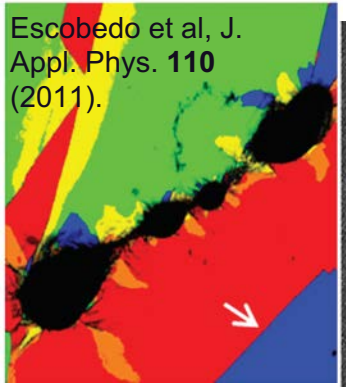


Lehtinen et al., *Scientific Rep.*, **8** (2018).

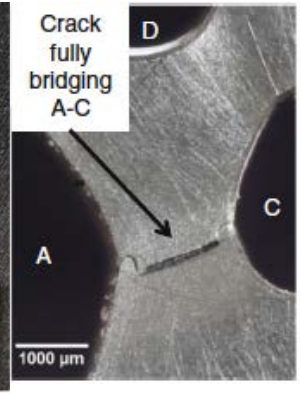
Ductile and Brittle Damage Mechanisms



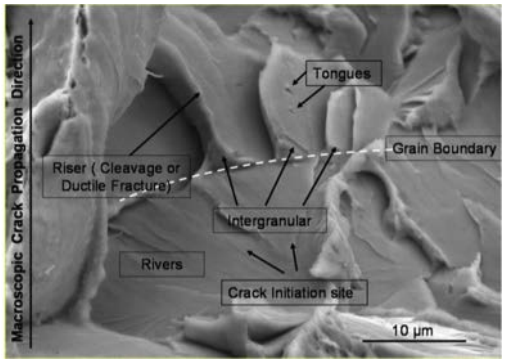
Escobedo et al, J. Appl. Phys. **110** (2011).


Escobedo et al, J. Appl. Phys. **110** (2011).

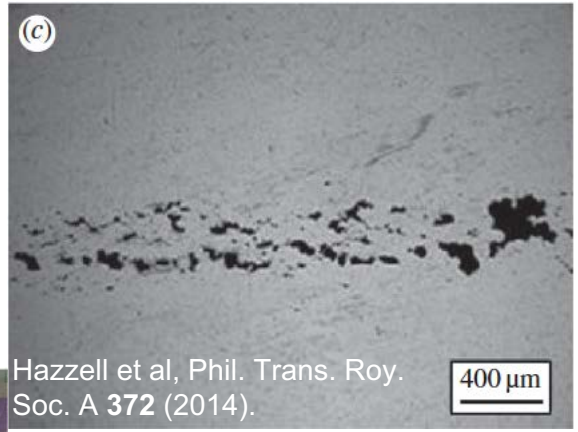
Boyce et al, Int. J. Frac. **186** (2014).



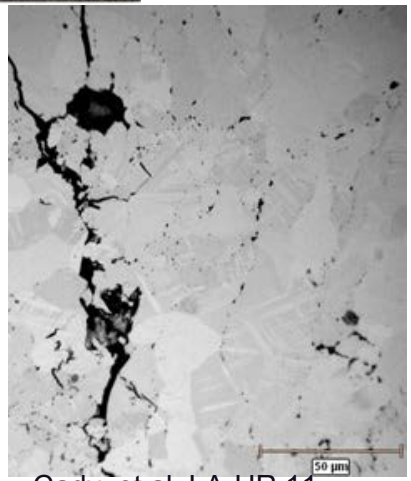
Escobedo et al, J. Appl. Phys. **110** (2011).



Pineau et al, Acta Mater. **107** (2016).



Hazzell et al, Phil. Trans. Roy. Soc. A **372** (2014).



Cady, et al. LA-UR 11-06976 (2011).

Boyce et al, Int. J. Frac. **198** (2016).

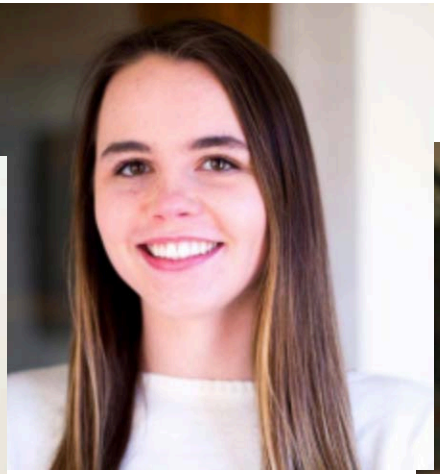
Refractory Multiple Principle Element Alloys (MPEAs)

Collaboration with UCSB

- **Multi-year collaboration with University of California, Santa Barbara**
- **UCSB Affiliate since Spring 2017**
  - Corresponded with 3 extended visits (~2 months) in Spring 2017, 2018, 2019.
  - Work with graduate students and postdocs, give guest lectures, seminars, and sit on thesis committees.
- **Dr. Irene Beyerlein's Group**

Irene Beyerlein

Shuozhi Xu

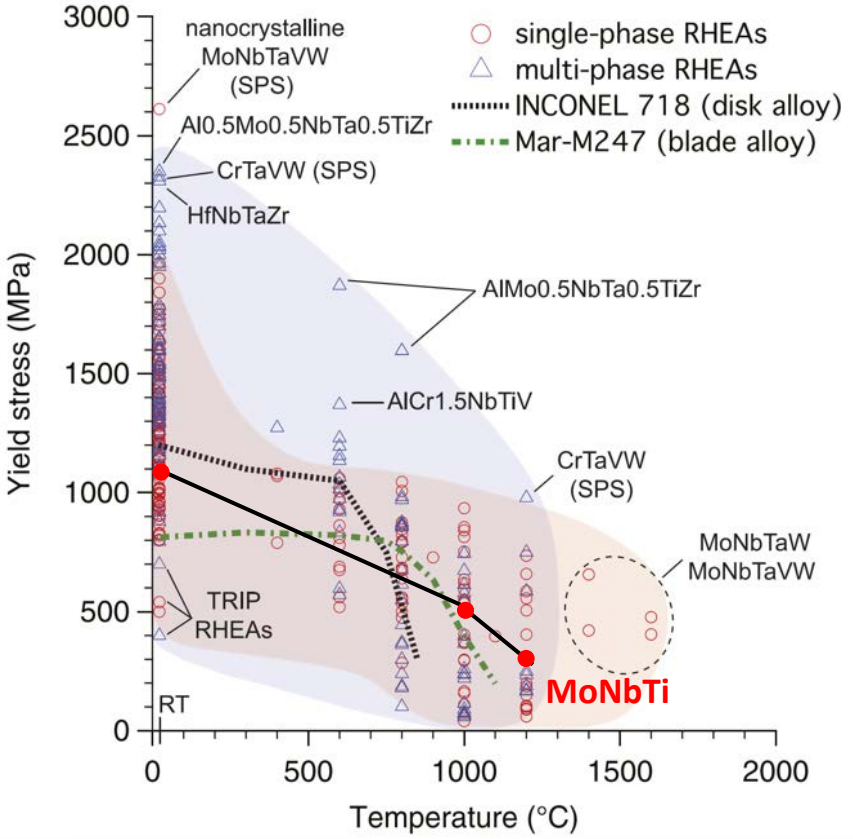


Lauren Smith

Claire Albrecht

Refractory MPEAs

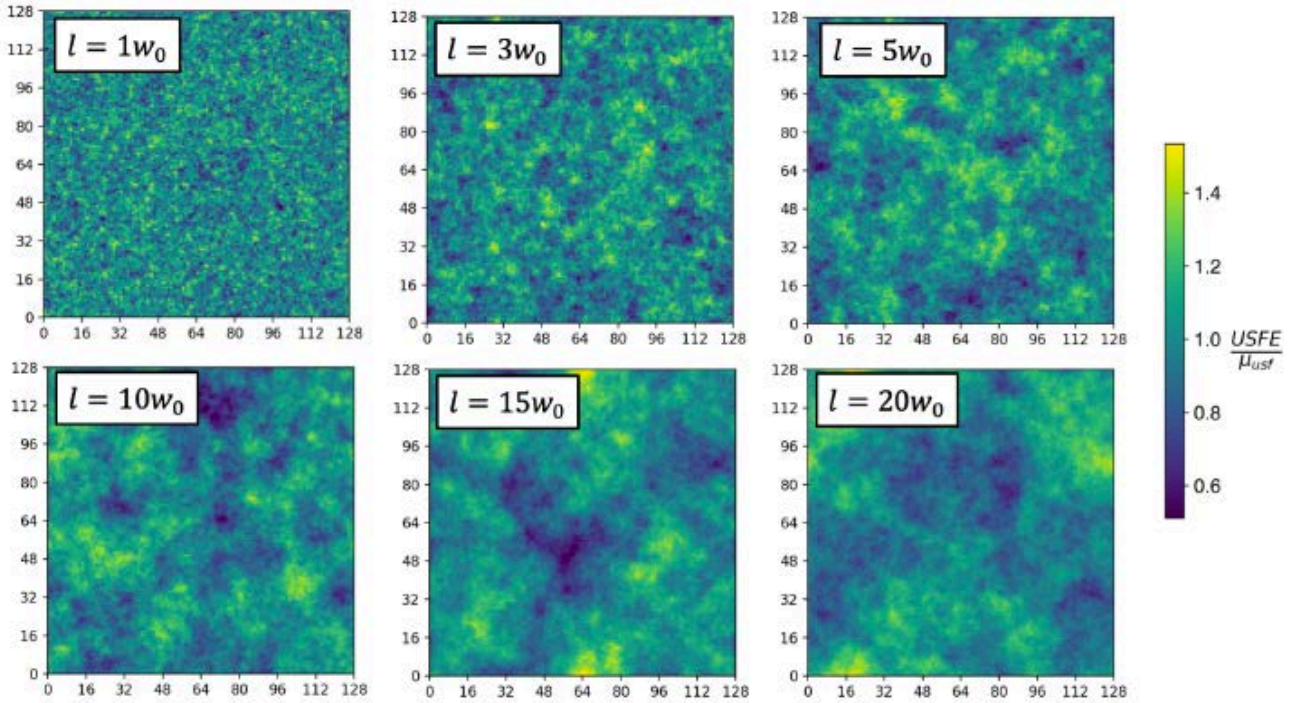
- **Disordered solid solutions with 3 or more elements in roughly equimolar concentrations**
  - Equimolar MoNbTi
- **Extraordinary mechanical properties**
  - High yield strength
  - High toughness
  - Specifically refractory MPEAs maintain their strength at elevated temperatures



Senkov et al., *J. Mater. Res.*, **33** (2018).
Senkov et al., *Acta Mater.*, **175** (2019).

Variation in Chemical Composition

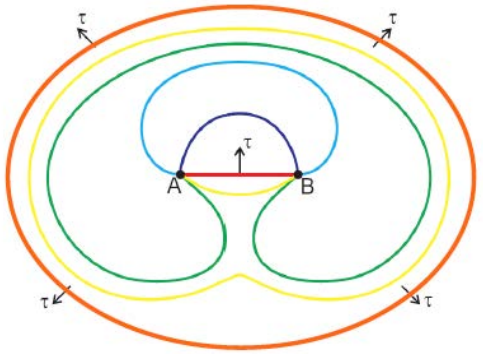
- **It is believed that there is some short range order on the order of nanometers**
  - Our correlation lengths range from ~0.5nm to 10nm

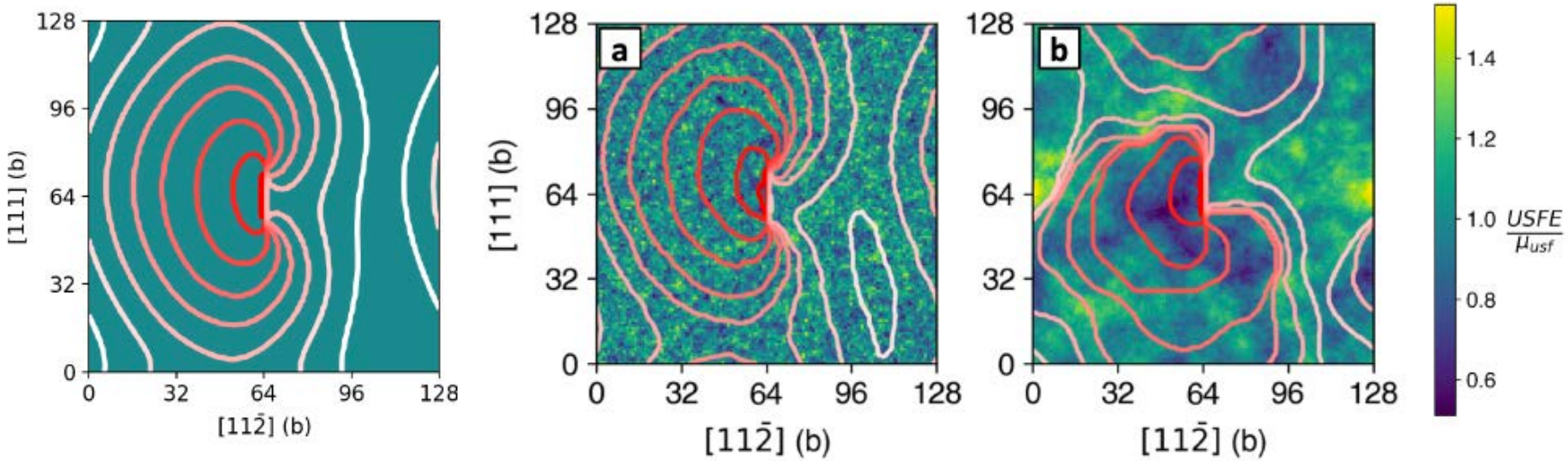


Smith, Su, Xu, Hunter and Beyerlein, *IJP* **134** 2020.

Effect of Short Range Order

- **Frank-Read Source**
  - We start to see ‘wavy’ dislocations
  - Waviness of the dislocation decreases as the correlation length decreases.

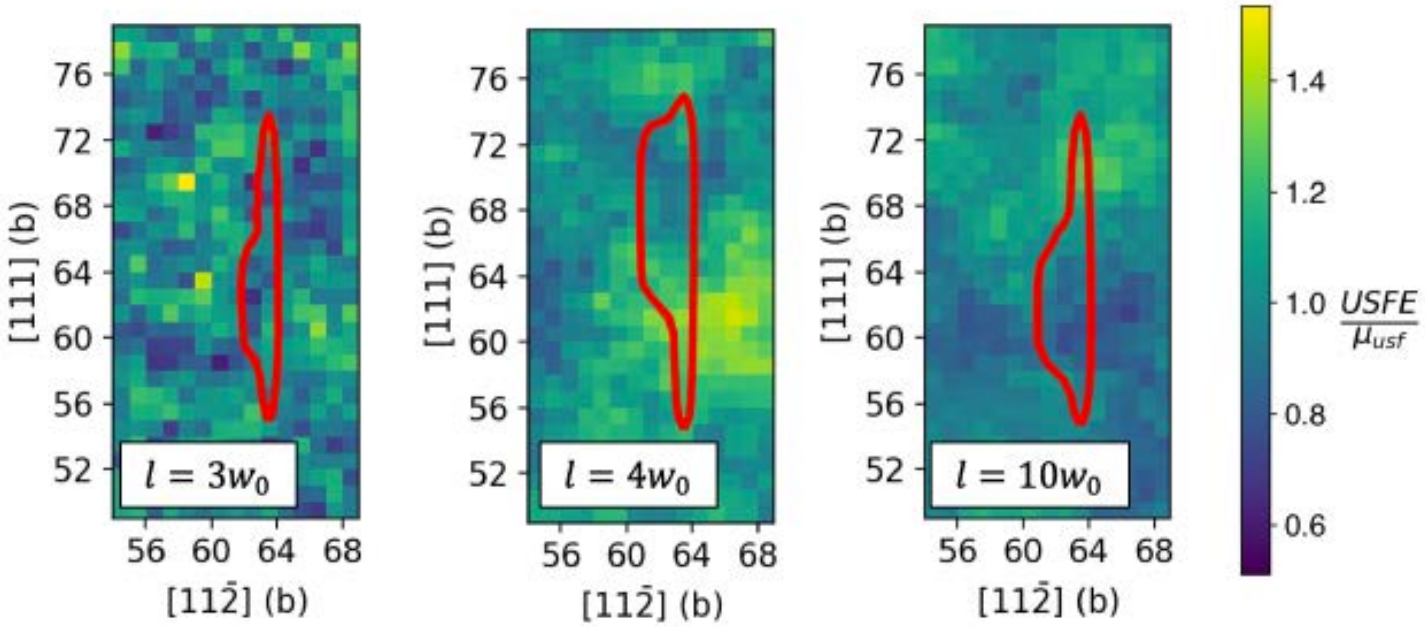




Smith, Su, Xu, Hunter and Beyerlein, *IJP* **134** 2020.

Kink-Pair Propagation Mechanism

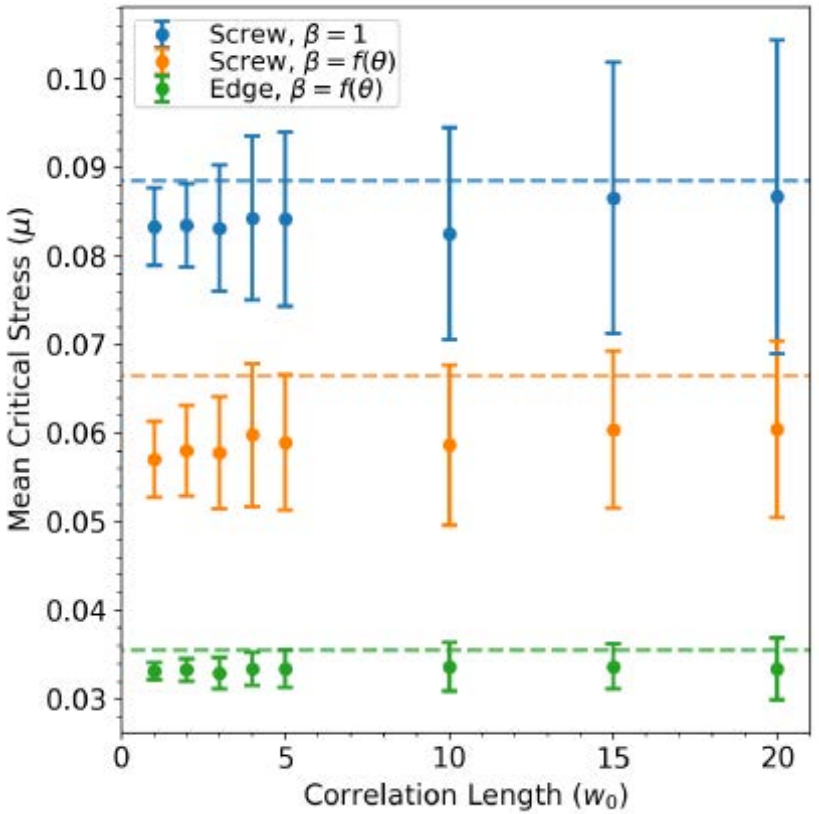
- **Initial segments that screw-type propagate through this mechanism.**
  - Dislocation segments move into low energy regions
  - Results in a decrease in the critical activation stress with respect to the homogeneous case.



Smith, Su, Xu, Hunter and Beyerlein, *IJP* **134** 2020.

Taking a Statistical Viewpoint

- **60 different surfaces at each correlation length**
  - In all cases, the mean critical stress falls below the corresponding homogeneous case
- **The mean stress is not significantly influenced by the correlation length, while the variance of the critical stress increases with correlation length.**

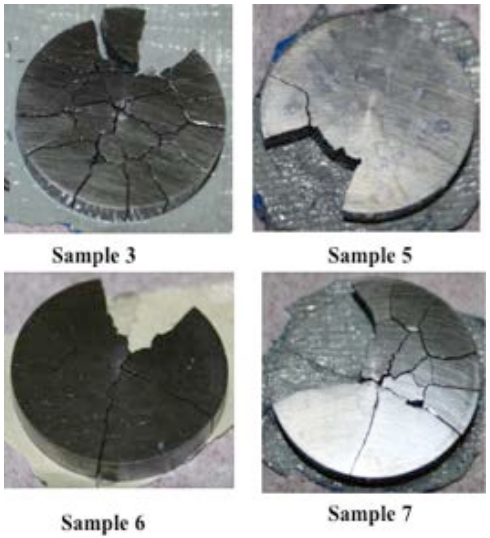


Smith, Su, Xu, Hunter and Beyerlein, *IJP* **134** 2020.

Failure in (Quasi-)Brittle Metals

(Quasi-)Brittle Materials

- **Have unique material behavior that is advantageous for engineering applications**
  - Infastructure, lightweight aircraft/automobile components
  - High strength-to-weight ratio and radiation resistant
  - Low intrinsic ductility and high anisotropy
    - Special loading, manufacturing, or fabrication conditions
- **Failure can be sudden and hard to predict**
  - Propagation and coalescence of heterogeneous micro-cracks

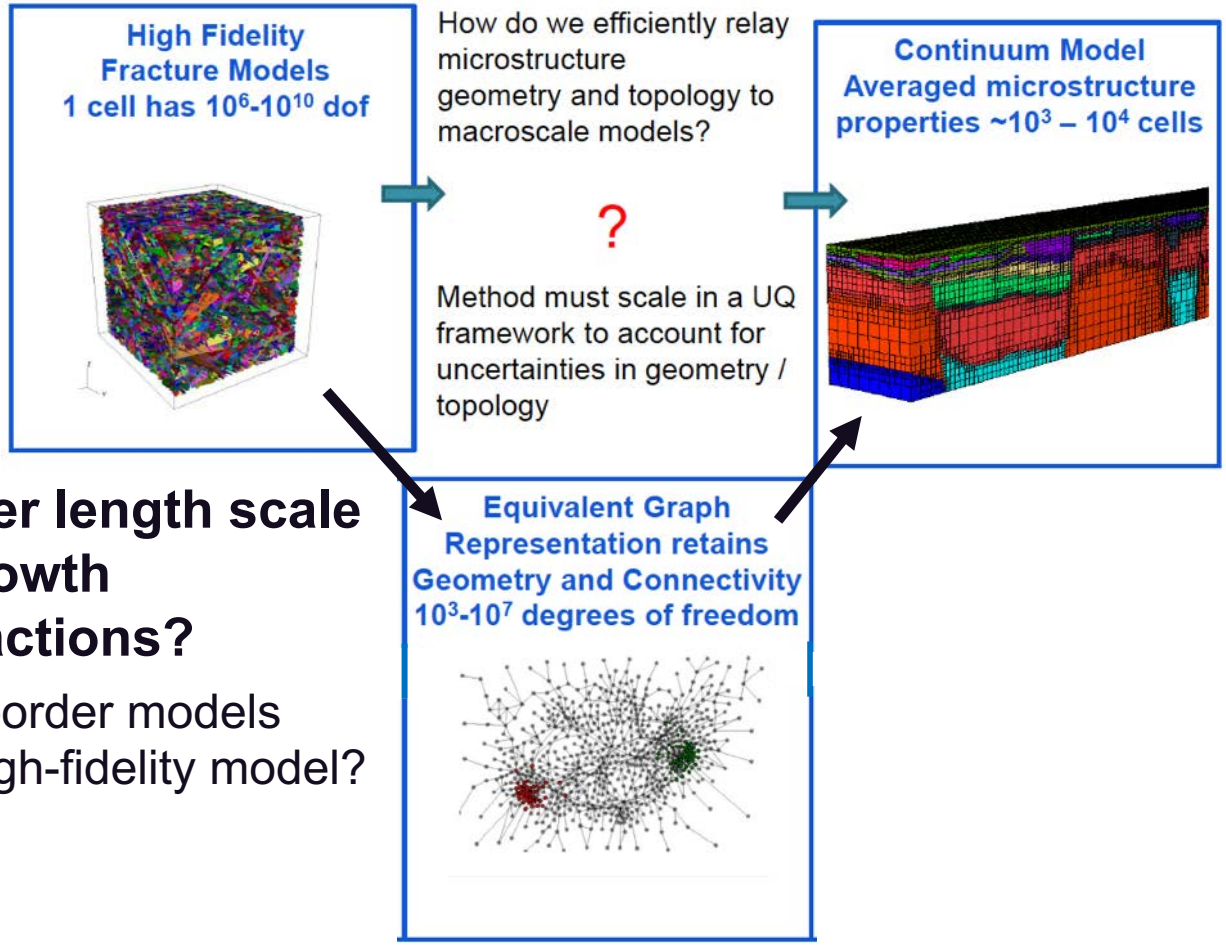


Kevin Larkin

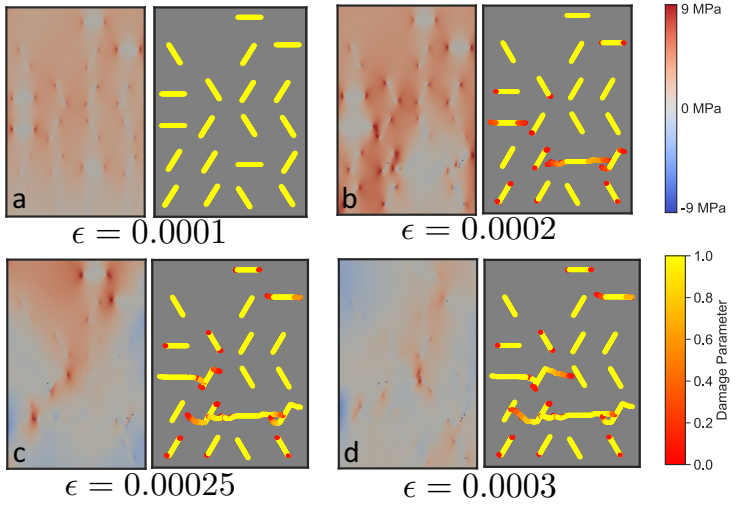
Blumenthal, et al. Shock Comp. Cond. Mat. (1997).
Cady, et al. LA-UR-11-06976 (2011).
Murr, et al. Mater. Sci. and Eng. A, **A151** (1992).

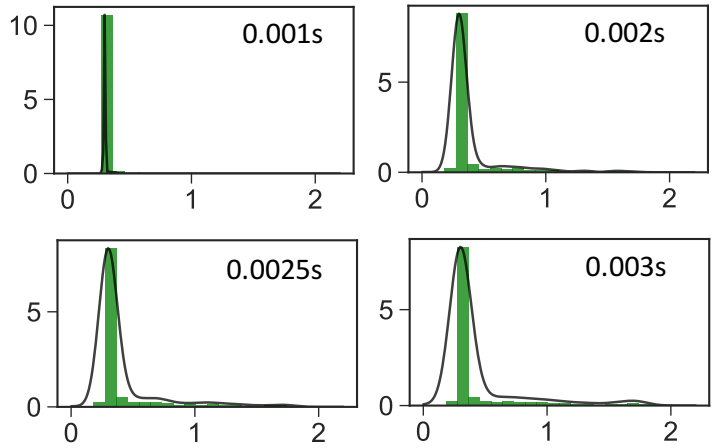
The problem of scaling up….

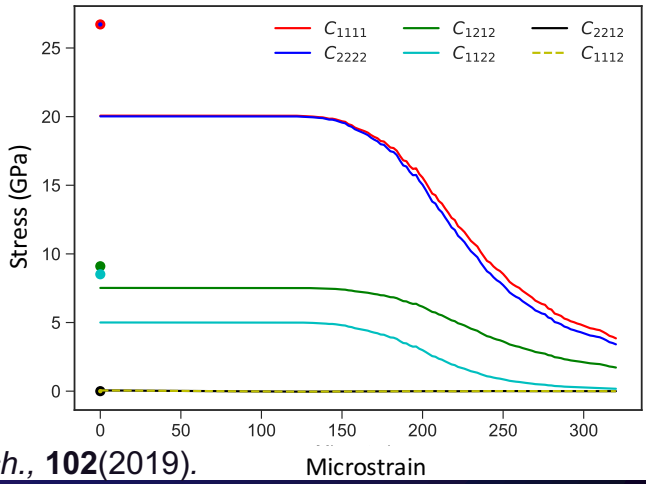
- **Representing the structure is computationally intensive**
  - Representing all possible crack orientations
- **How do we inform larger length scale models about crack growth coalescence and interactions?**
  - Can we develop reduced-order models (ROMs) to emulate the high-fidelity model?

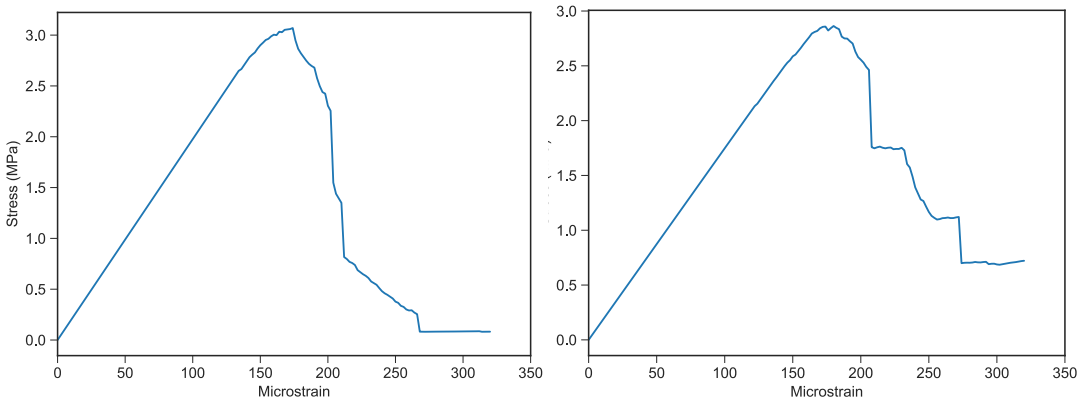


Bridging Scales



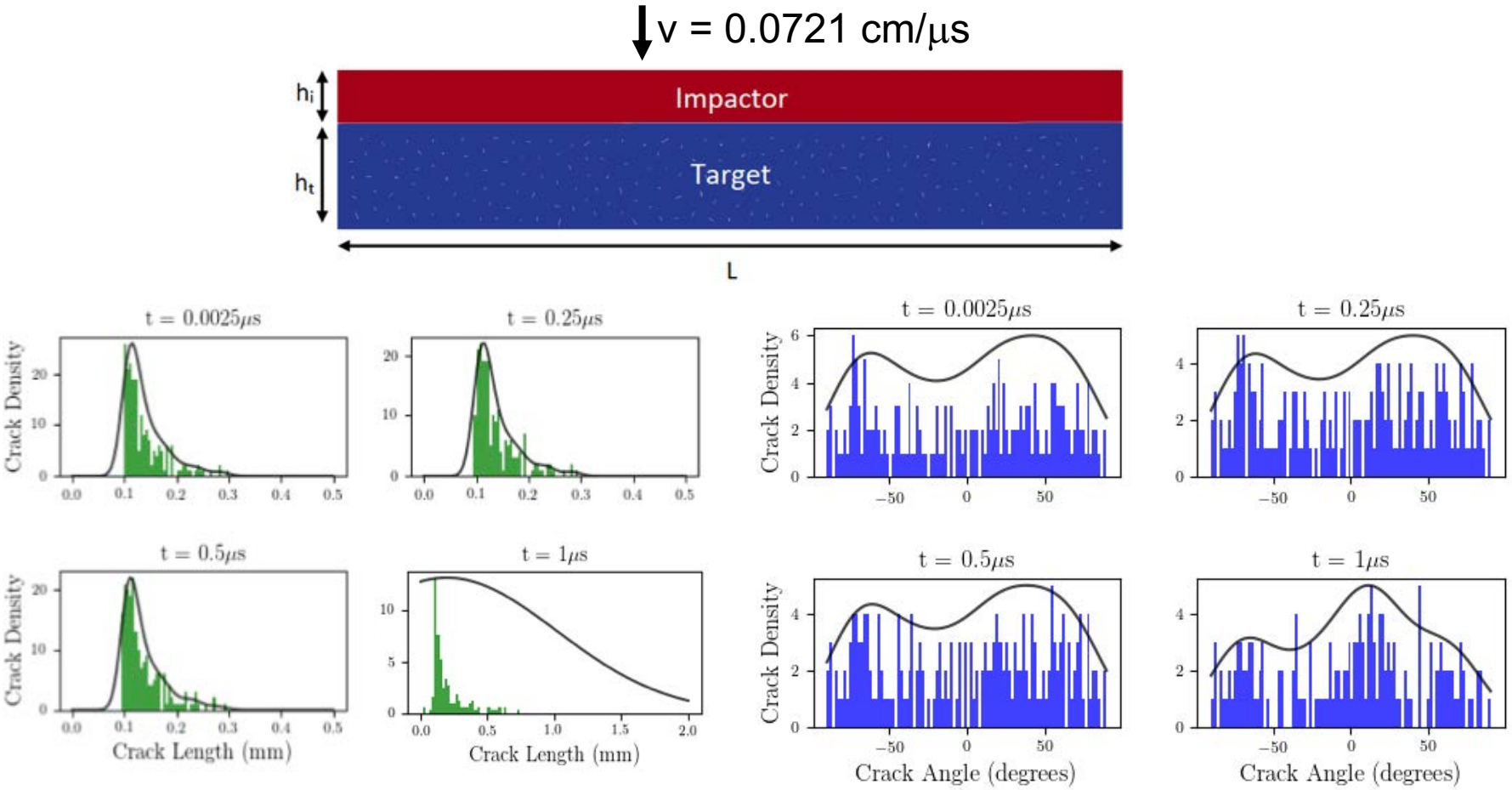






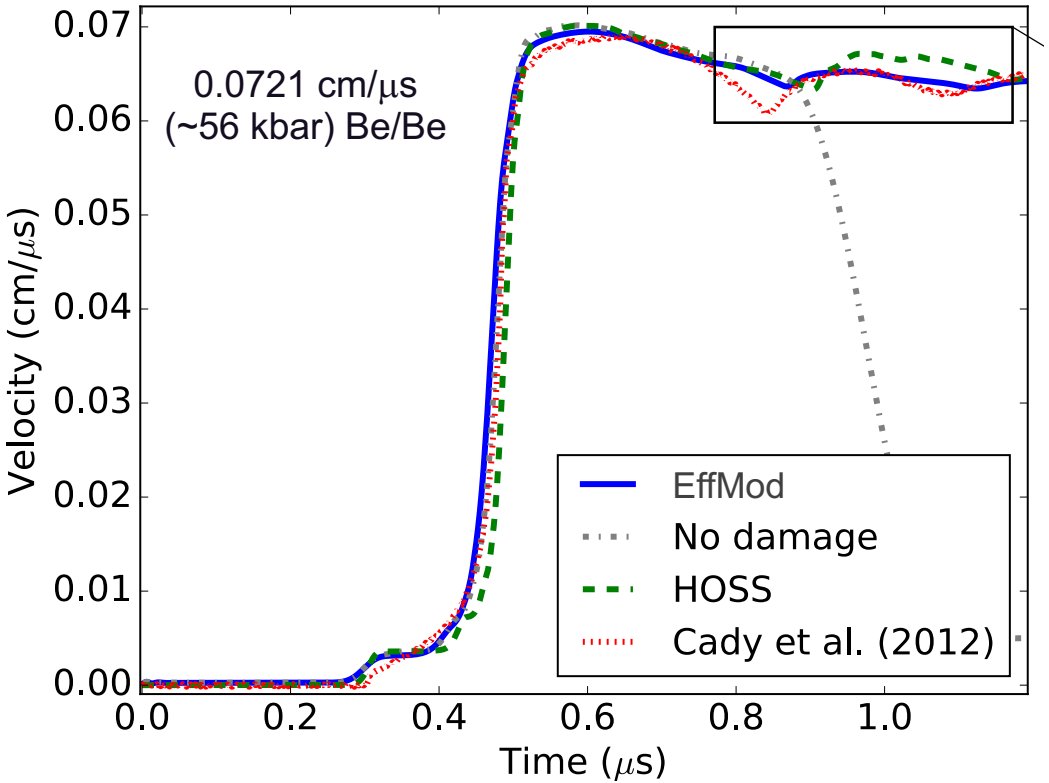
Vaughn, Kononov, Moore, Rougier, Viswanathan, Hunter, *Theo. and App. Fracture Mech.*, **102**(2019).

Generating Probability Density Functions (PDFs)

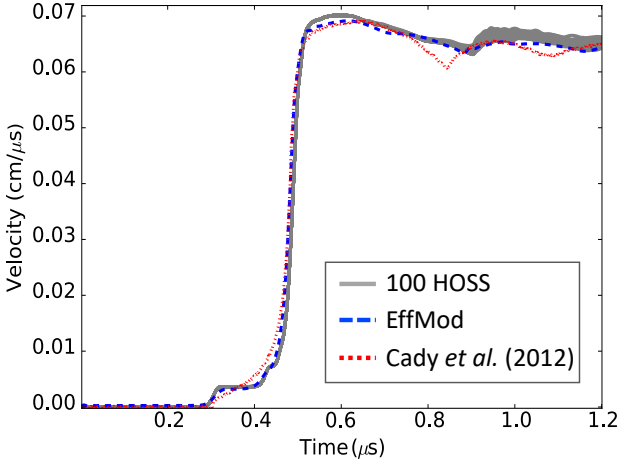


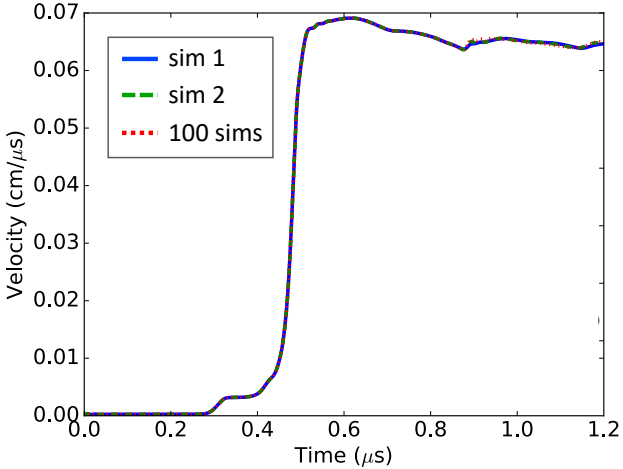
Larkin, Rougier, Chau, Srinivasan, Abdelkefi, Hunter, *JMPS* **138** (2020).

Results



Cady, et al. LA-UR-11-06976 (2011).

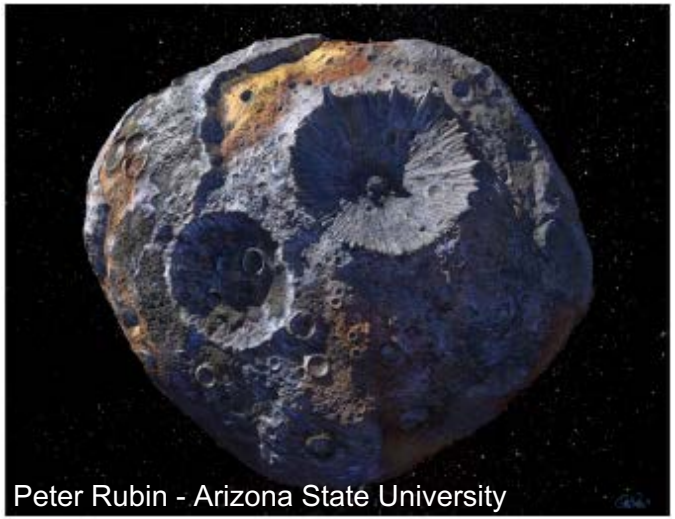




Predicting the Composition of Asteroid 16 Psyche

Asteroid 16 Psyche

- **Upcoming NASA Mission to Psyche: Journey to a Metal World**
  - Launch 2022, Psyche Arrival 2026, Orbit for 21 months.
- **Largest M-type (metallic) asteroid in the Main Asteroid Belt**
  - First mission of its kind to visit a metallic body, rather than one composed of ice or rock.
  - Could be the remnant of a differentiated planet core – unique look at planet formation
- **What is Psyche made of?**
  - Bulk density estimates: 1.4 ± 0.3 – 4.5 ± 1.4 g/cm^3

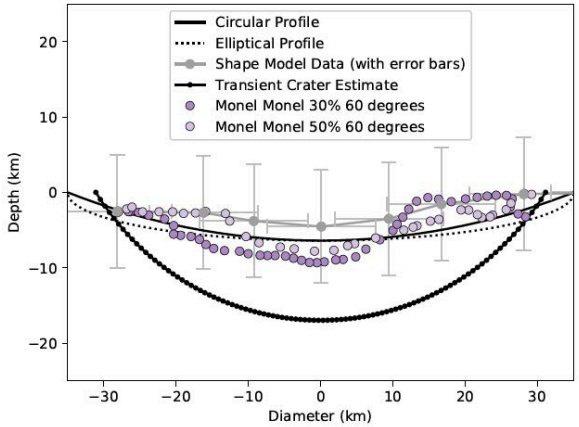

Peter Rubin - Arizona State University

Lupishko, *Solar Sys. Res*. **40** (2006).
Oh et al. *Joint Pro. Conf.* (2016).

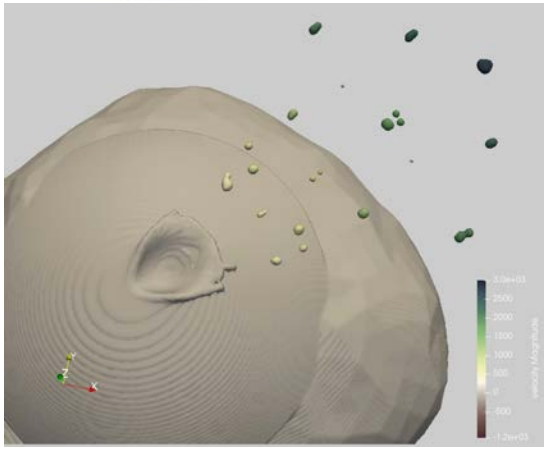
Wendy Caldwell

Modeling Impact Craters

- **Psyche has two large impact structures in the Southern hemisphere**
  - Diameters: 53±15 km and 67±15km
  - Depth: 6.4±0.64 km
- **What is Psyche's Composition?**
  - Type of material – Ni, Fe, Monel
  - Amount of porosity – micro vs. macro

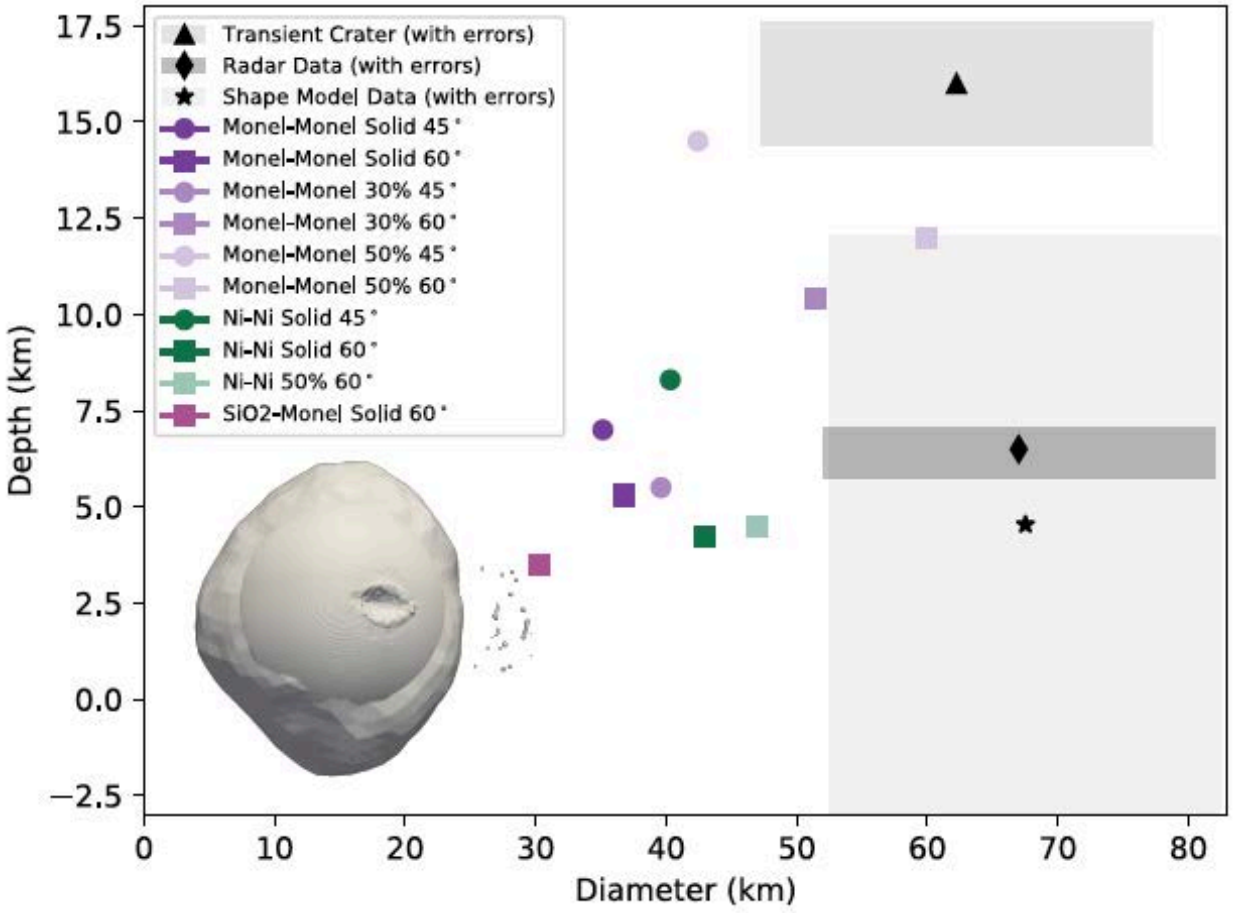


Shepard et al. *Icarus* **281** (2017).



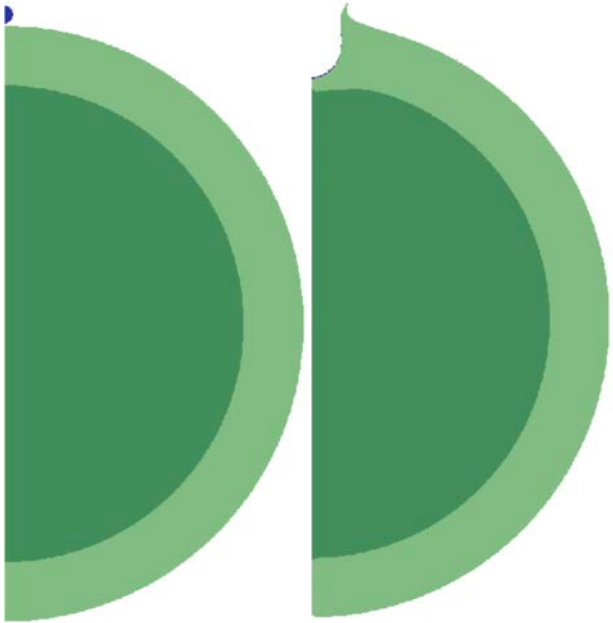
Caldwell, Hunter, Plesko, Wirkus, *Icarus* **351** (2020).

Larger Crater: 3D Results



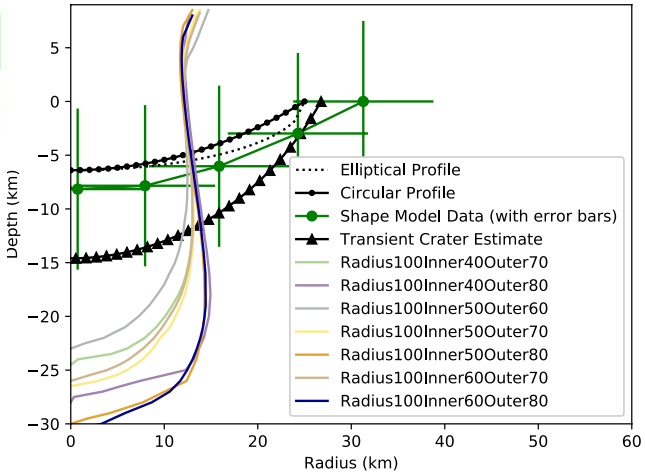
Caldwell, Hunter, Plesko, Wirkus, *Icarus* **351** (2020).

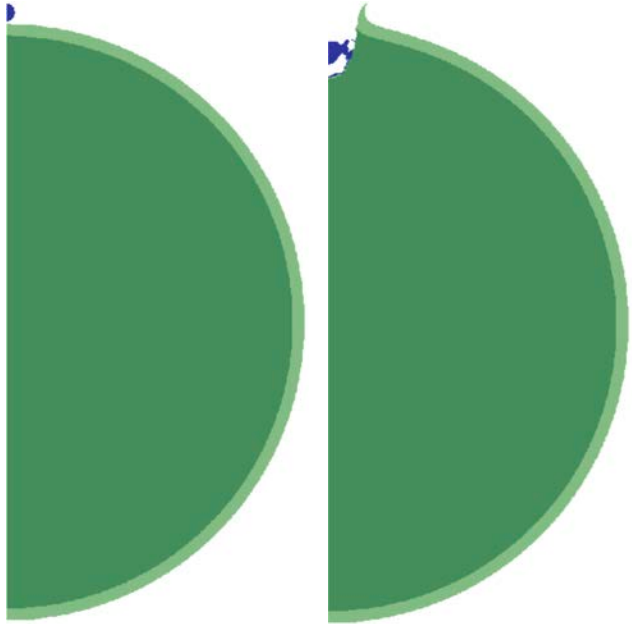
Micro vs. Macro porosity – Layers



Inner radius = 100 km with 50% porosity

Outer radius = 125 km with 60% porosity



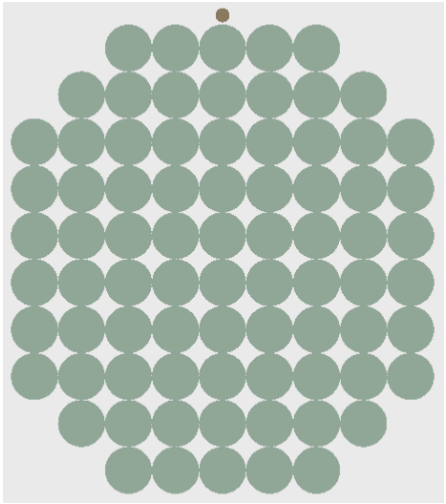


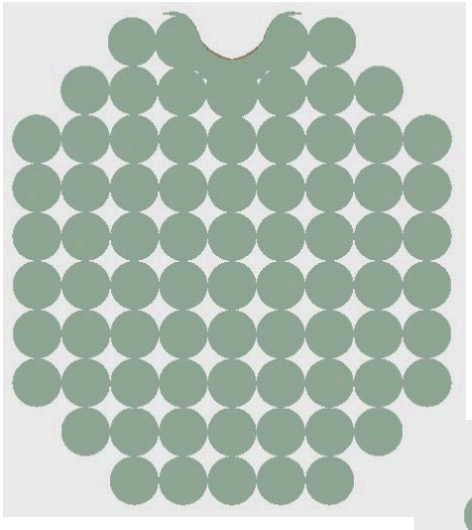
Inner radius = 120 km with 50% porosity

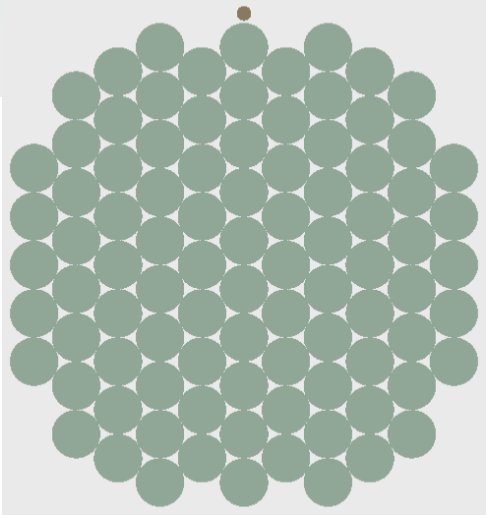
Outer radius = 5 km with 70% porosity

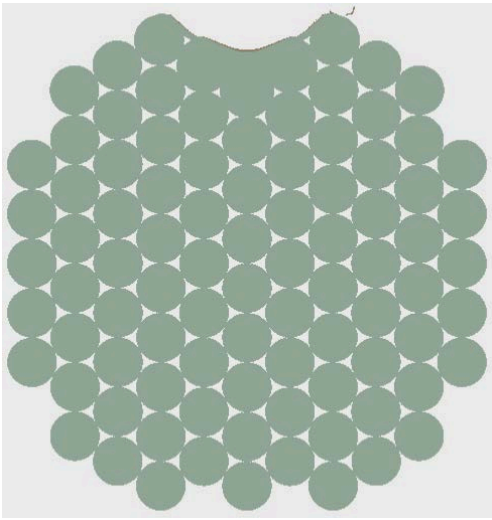
Caldwell, Hunter, Plesko, *in prep.*

Micro vs. Macro porosity – Rubble Piles









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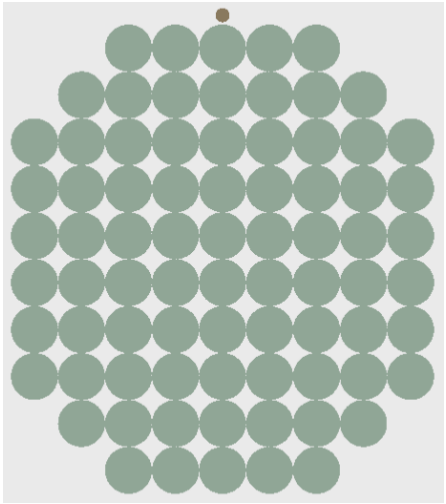
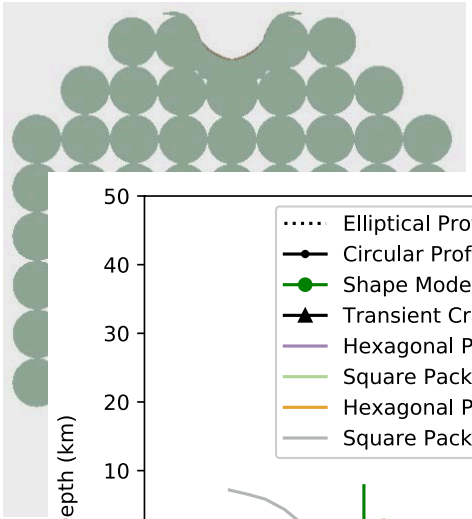
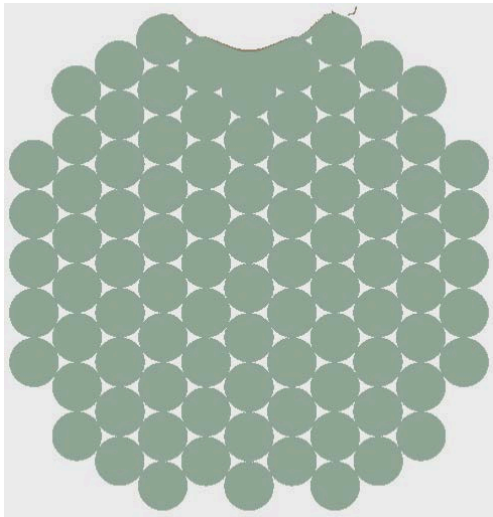
Micro vs. Macro porosity – Rubble Piles







Caldwell, Hunter, Plesko, *in prep.*

Foundation is key…

- **I've come a long way, thanks to a strong foundation**
  - Thanks to institutions committed to providing their students with a strong educational background and also future opportunities.
  - Thanks to individuals who have taken extra time to invest in the success of the people around them.
- **I hope to help others build a strong foundation**

IMS Institute for Materials Science Los Alamos

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Collaborators and Colleagues

- Los Alamos National Laboratory
  - D. J. Luscher
  - Enrique Martinez Saez
  - Nithin Mathew
  - Wendy Caldwell
  - Cathy Plesko
- University Collaborators
  - Kaushik Dayal – Carnegie Mellon University
  - Irene Beyerlein – University of California, Santa Barbara
  - Abdu Abdelkefi – New Mexico State University
- Postdoctoral Researchers
  - Kevin Larkin – Los Alamos National Laboratory
  - Shuozhi Xu – University of California, Santa Barbara
  - Yanqing Su - University of California, Santa Barbara
- Graduate Students
  - Jade Peng – Carnegie Mellon University
  - Lauren Smith– University of California, Santa Barbara
  - Claire Albrecht – University of California, Santa Barbara

Questions?