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Sandia National Laboratories

BCC Ta single crystals during Taylor impact

Using a coupled dislocation dynamics and finite element model

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Multiscale Materials Modeling

Wednesday, October 5th, 2022

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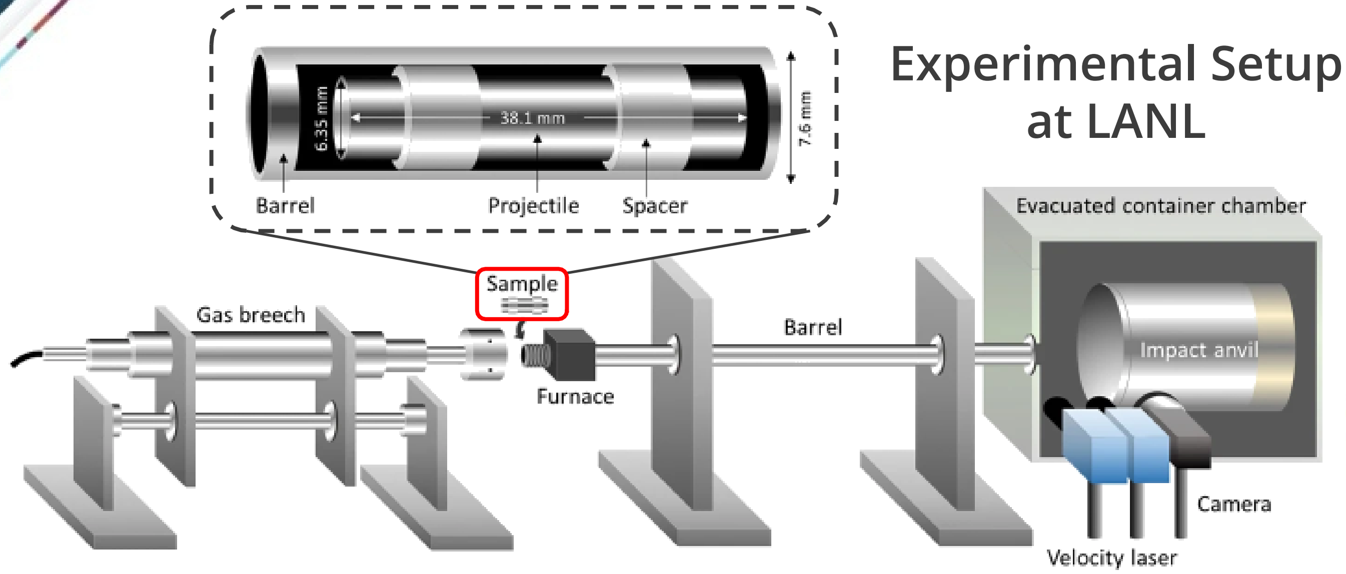
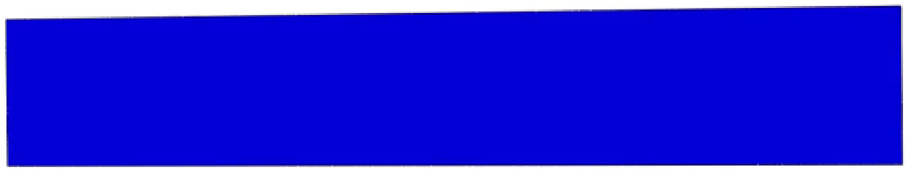
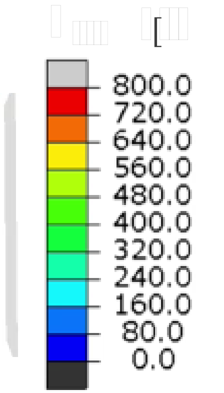
Taylor impact testing: a simple and robust technique to study dynamic behaviors

Experimental Setup at LANL



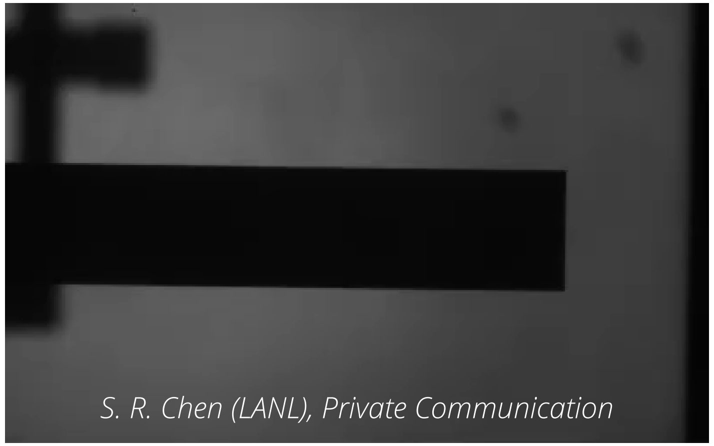
FEM Approximation

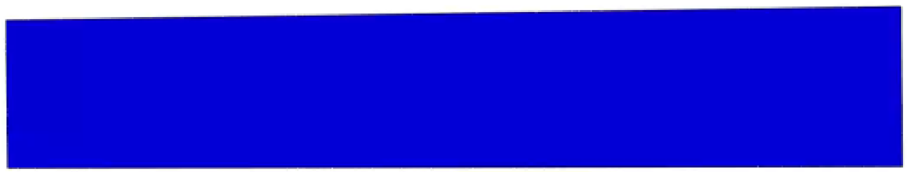


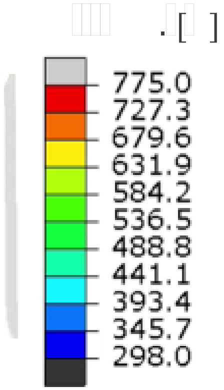


Large stress gradients!

Polycrystalline Ta



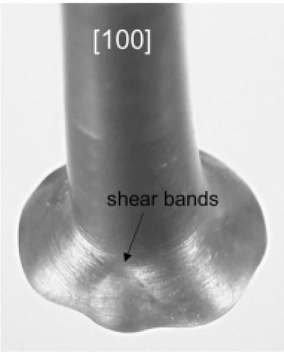


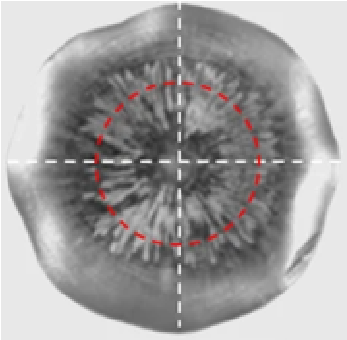


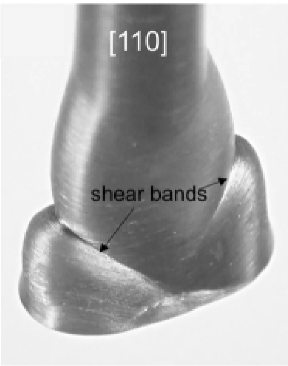
Large temperature gradients!
(ΔT ~ 500 K)

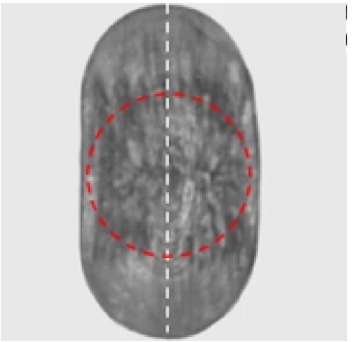
H. Lim, et al., Scientific Reports (2018)

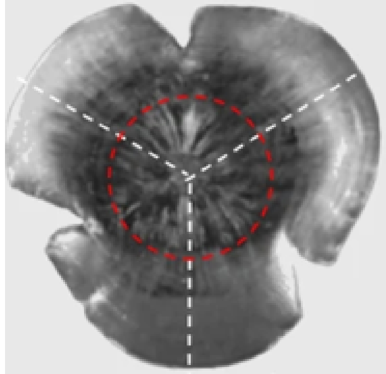
Ta single crystals display strong anisotropy



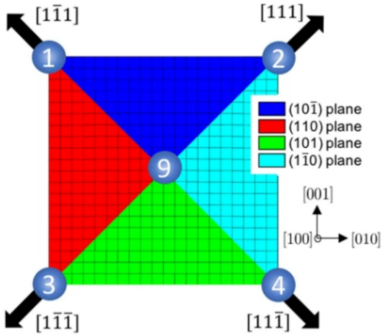




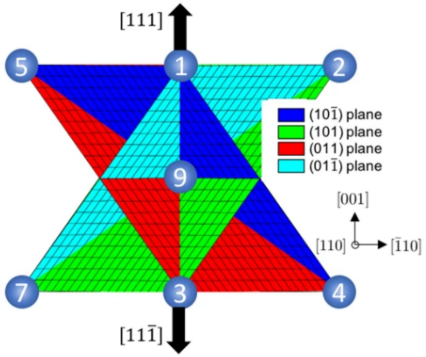




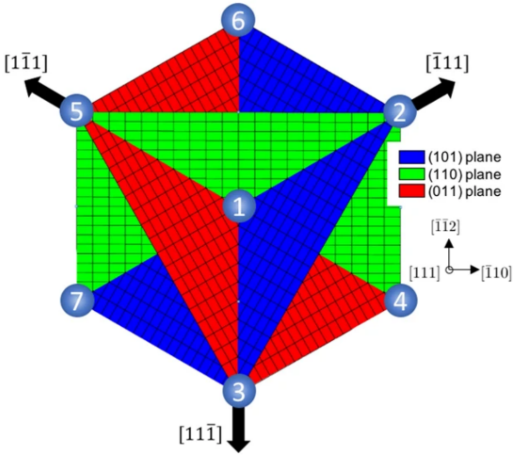
Four-fold symmetry

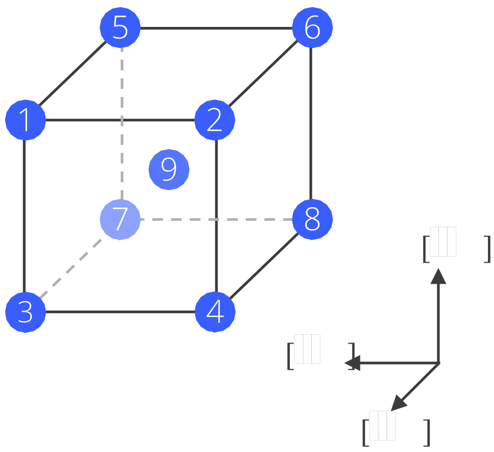


Two-fold symmetry



Three-fold symmetry

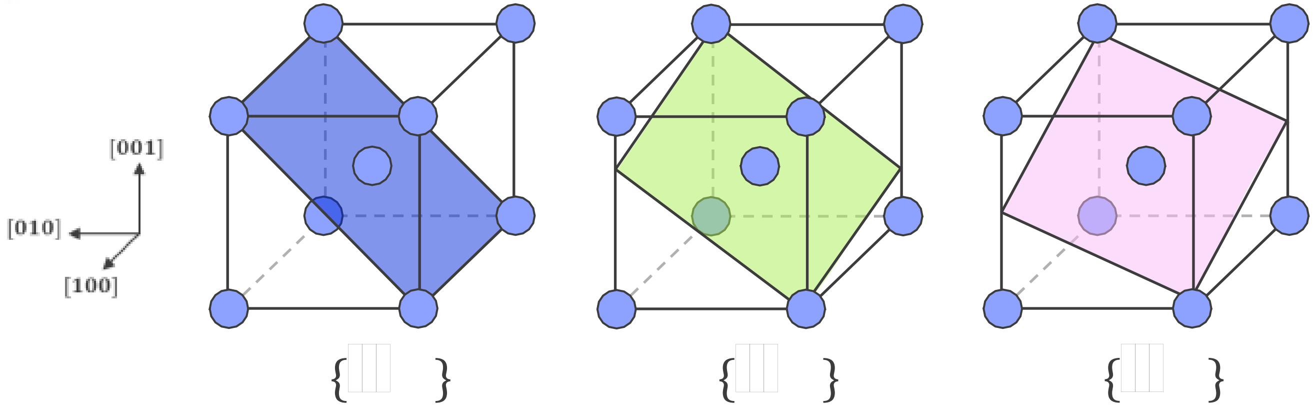




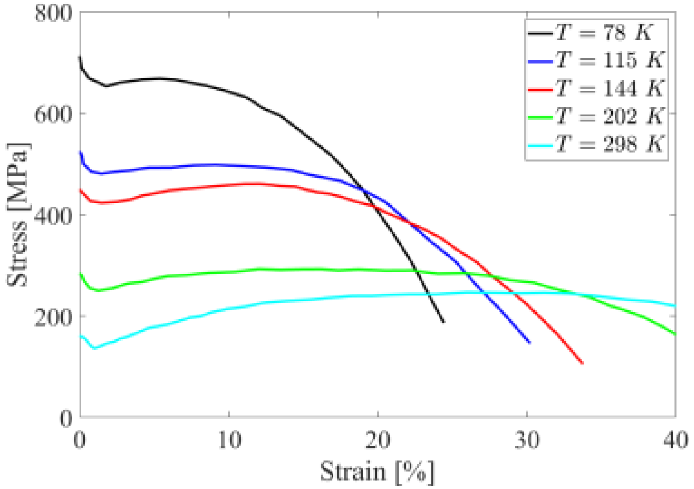
H. Lim, et al., Scientific Reports (2018)

Modeling BCC metals & recent efforts

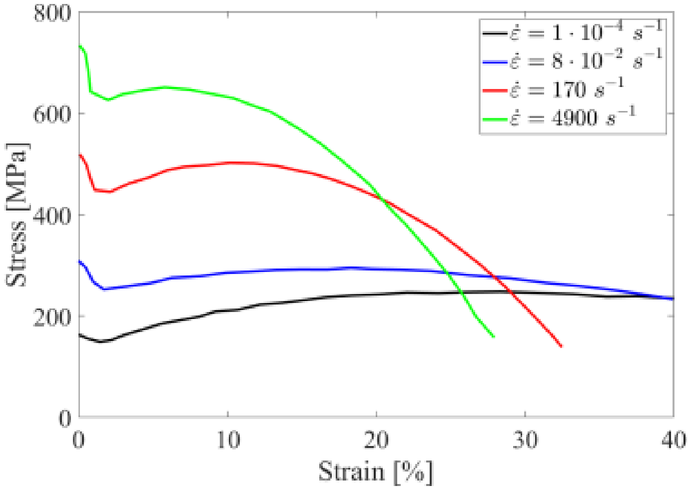
Many possible slip systems



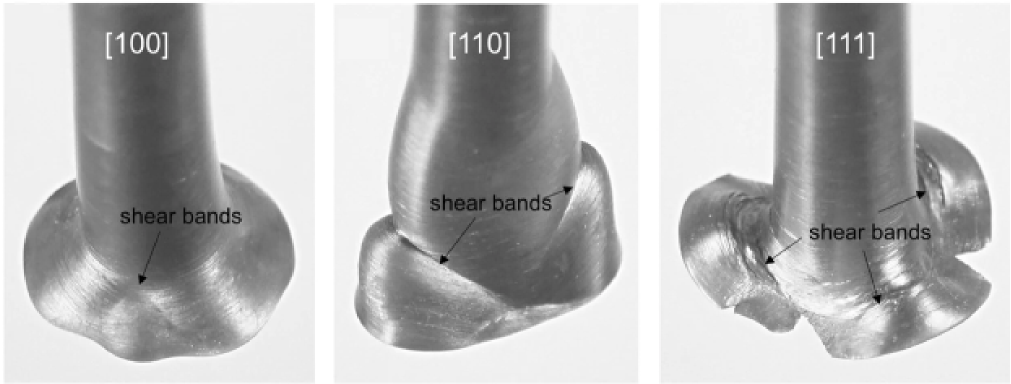
Temperature dependence



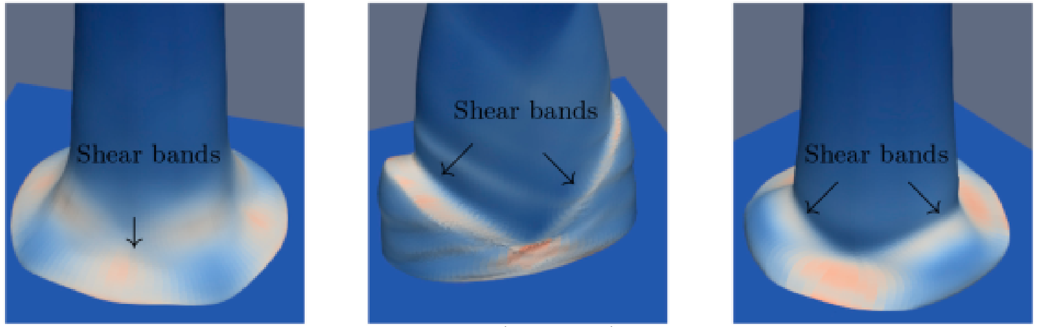
Strain-rate dependence



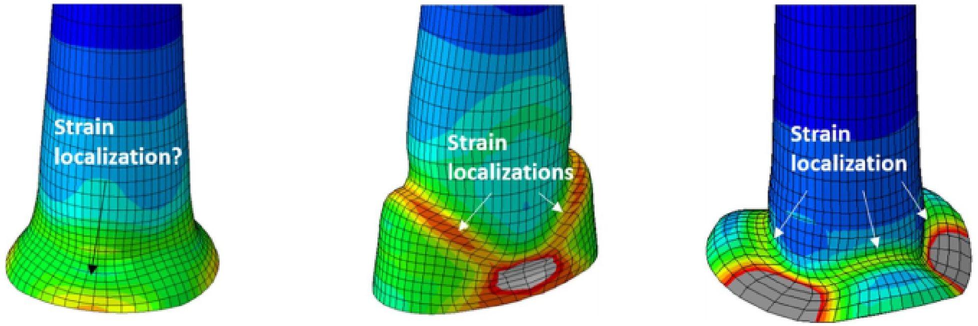
K.G. Hoge and A.K. Mukherjee, J. Mater. Sci. (1977)



H. Lim, et al., Scientific Reports (2018)

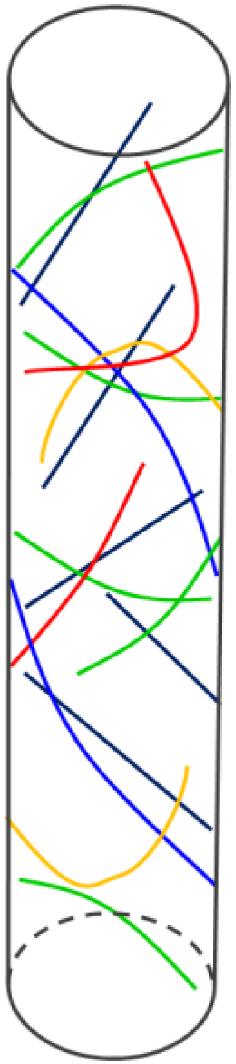


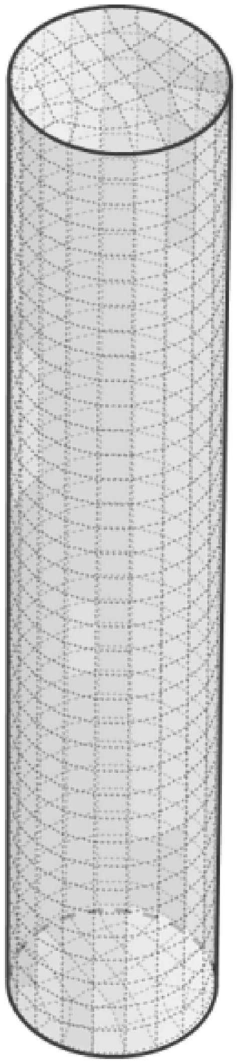
T. Nguyen, et al. Int. J. Plast. (2021)



Z. Feng, et al. Int. J. Solids Struct. (2022)

Dislocation dynamics vs. Finite element method





Dislocation Dynamics (DD)

- Detailed defect interactions
- Limited geometries
- Stationary geometry
- Small deformation

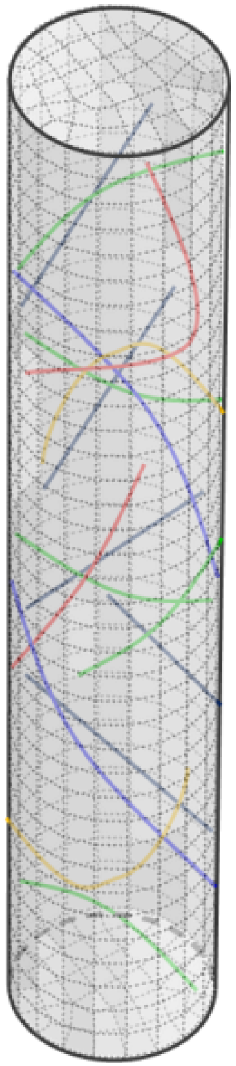
Finite Element Method (FEM)

- No microstructural information
- Any arbitrary geometry
- Evolving geometry
- Large deformation
- Multi-physical phenomena

Dislocation dynamics + Finite element method

<u>Defect dynamics element method (DDEM)</u>

- Detailed defect interactions
- Any arbitrary geometry
- Evolving geometry
- Large deformation
- Multi-physical phenomena

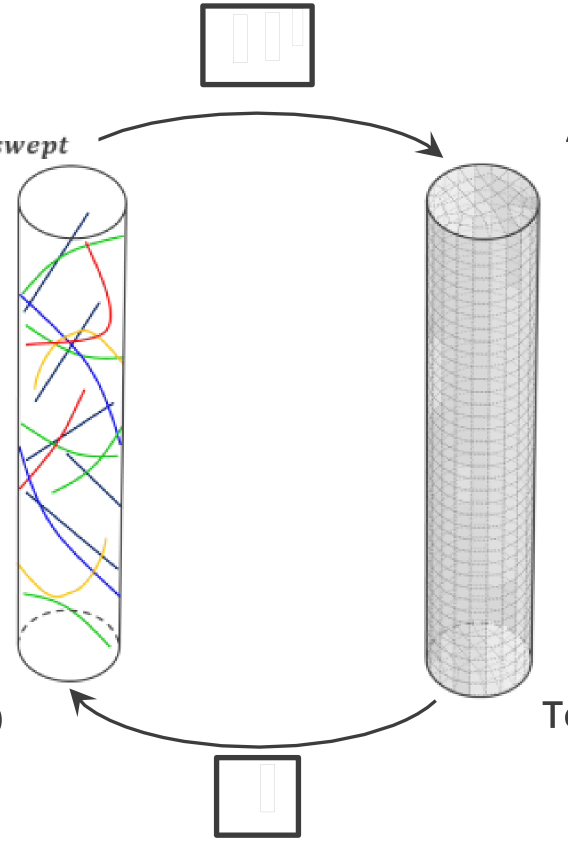


P.C. Nguyen et al. (To Be Submitted)

Defect dynamics element method (DDEM)

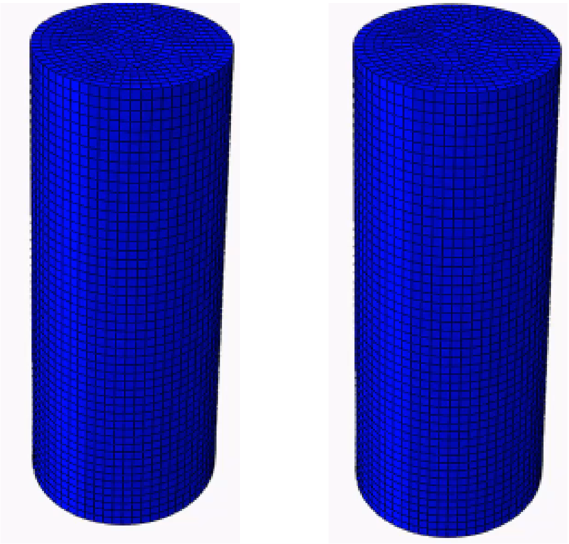
Concurrent Coupling

$$\Delta\varepsilon^P = \frac{b \otimes n + n \otimes b}{2\Omega} \Delta A_{swept}$$



Topology changes

Uniaxial Microcompression



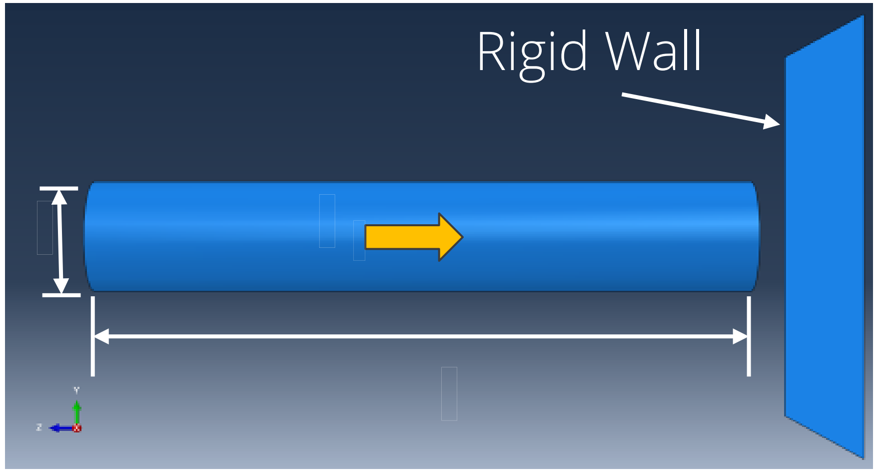
M. Uchic et al., Science (2004)

P.C. Nguyen et al. (To Be Submitted)

Modeling Taylor impact using DDEM

Model setup (*Ta*):

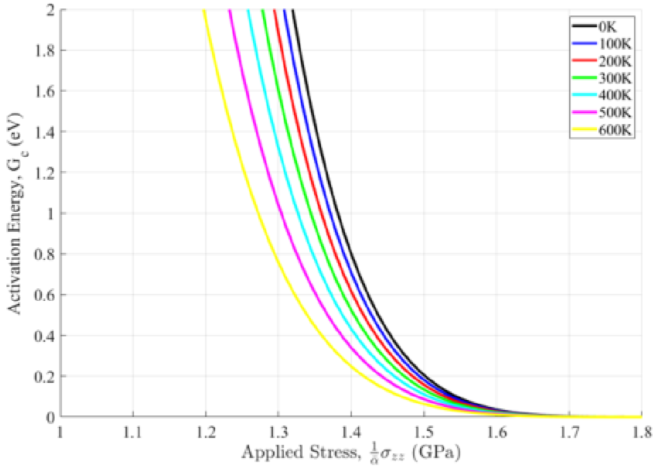
- Sample dimensions: *D ~ 1.6 μm, L ~ 9.5 μm*
- Initial velocity: v_0 = *150 m/s*
- Slip systems: {110}/<111>, {112}/<111>



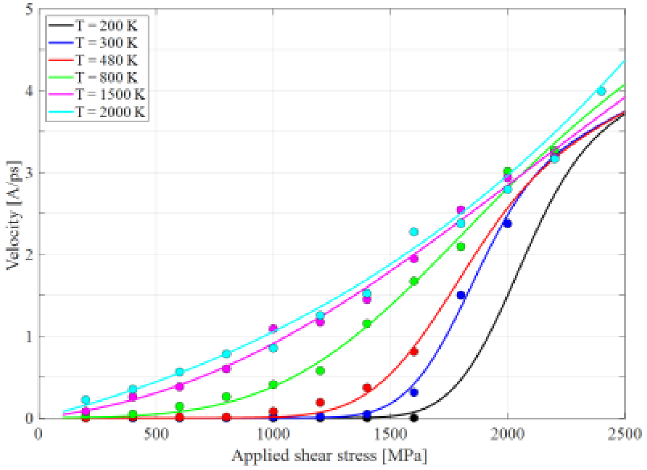
Temperature dependence:

- Heat from plastic dissipation (adiabatic)
- Dislocation mobility law – $v(\boldsymbol{\sigma}, \boldsymbol{T})$
- Dislocation nucleation – $G_c(\boldsymbol{\sigma}, \boldsymbol{T})$

Dislocation nucleation G_C

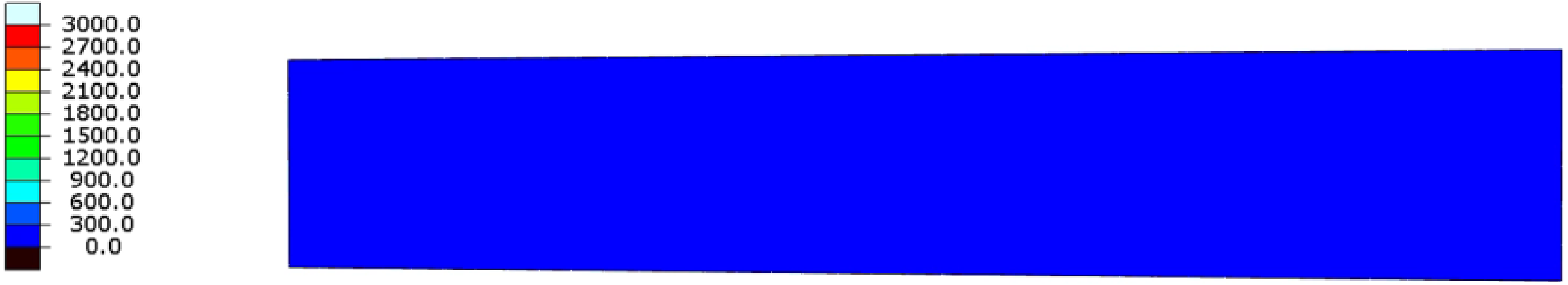


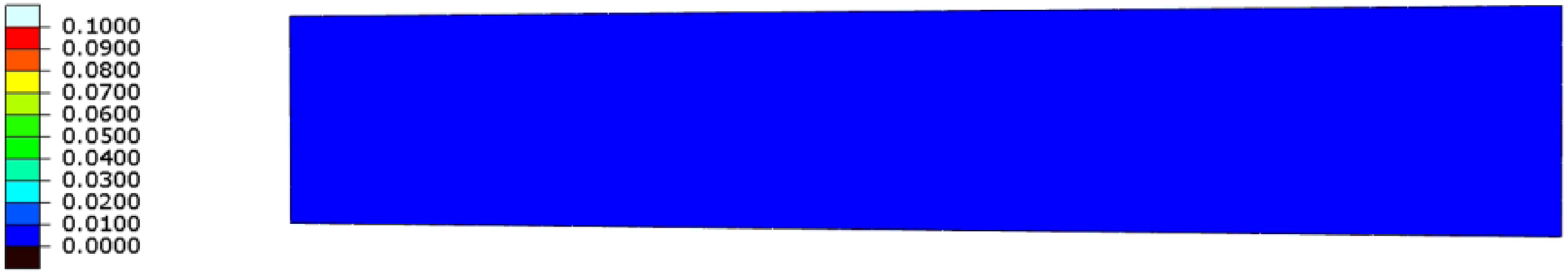
Screw dislocation velocity

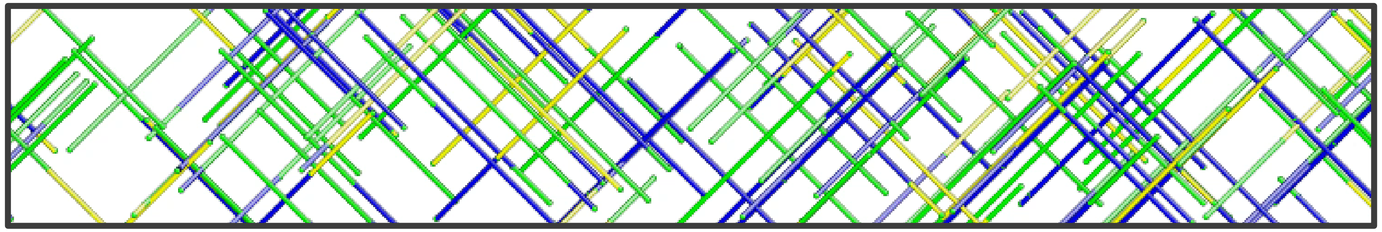


N.K. Aragon et al., Materialia (2021)

DDEM Results

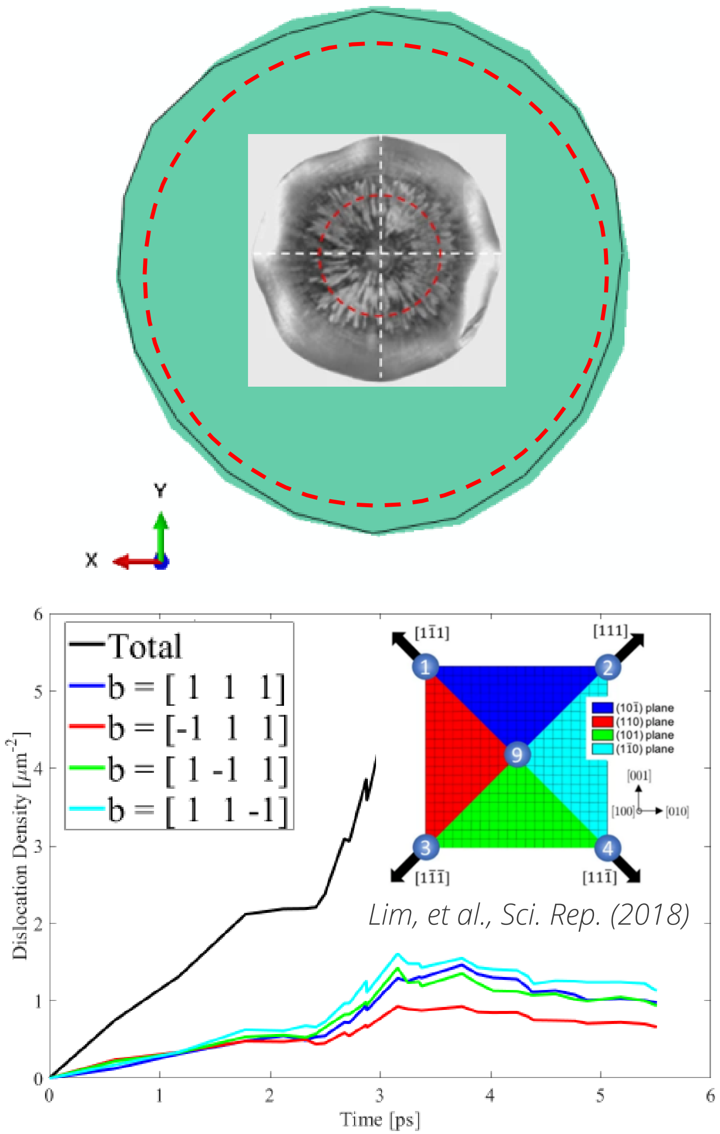




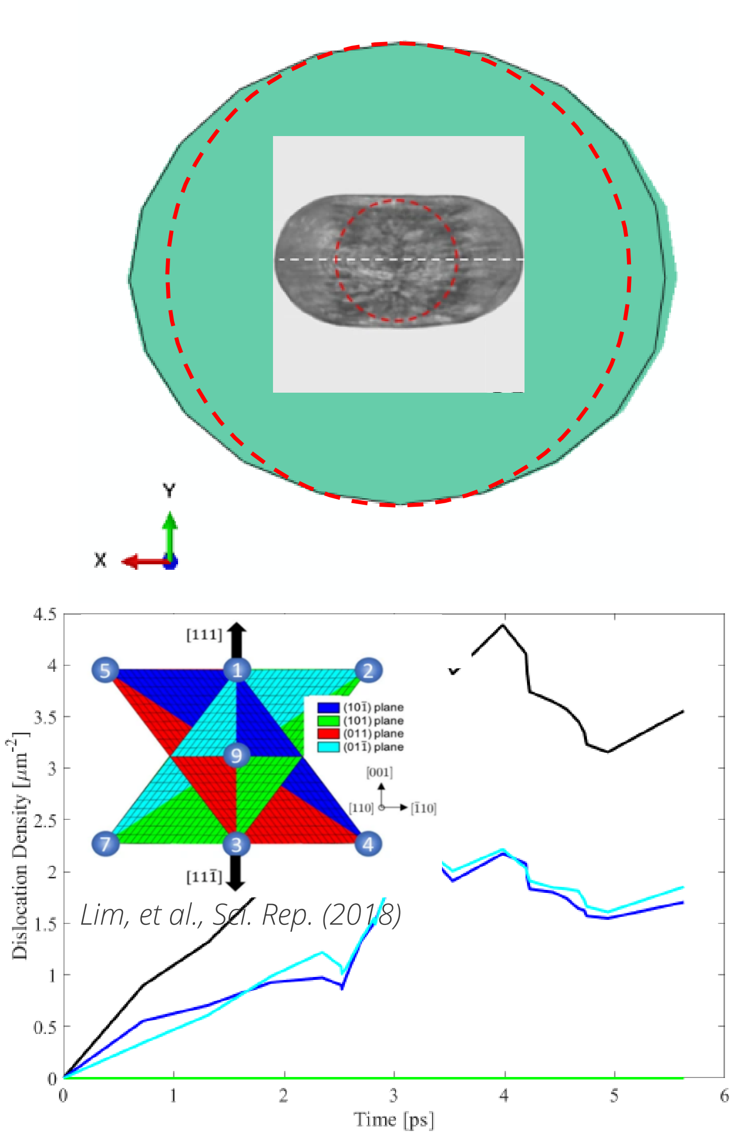


Dislocation localization at the impact foot causes stress to relax with limited propagation

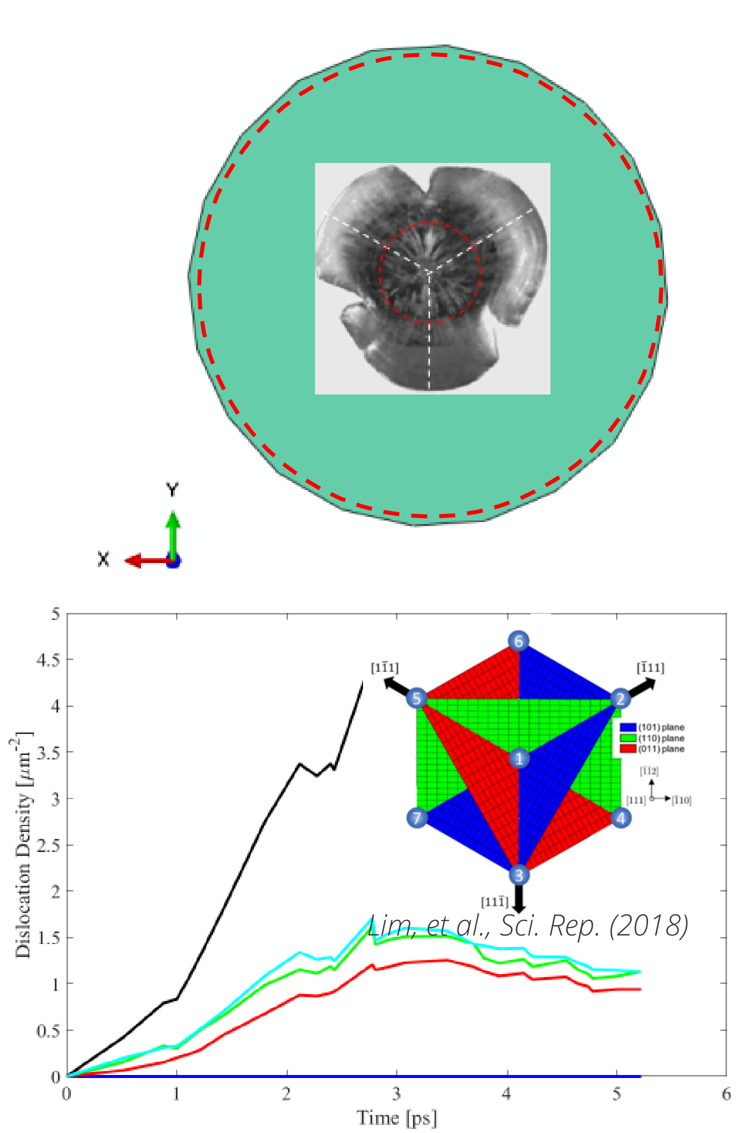
DDEM Results – Anisotropy



Lim, et al., Sci. Rep. (2018)



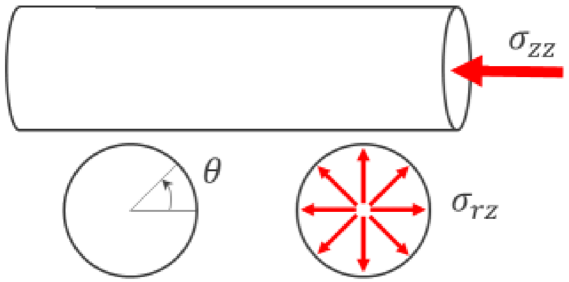
Lim, et al., Sci. Rep. (2018)



Lim, et al., Sci. Rep. (2018)

Anisotropy

Resolved Shear Stress

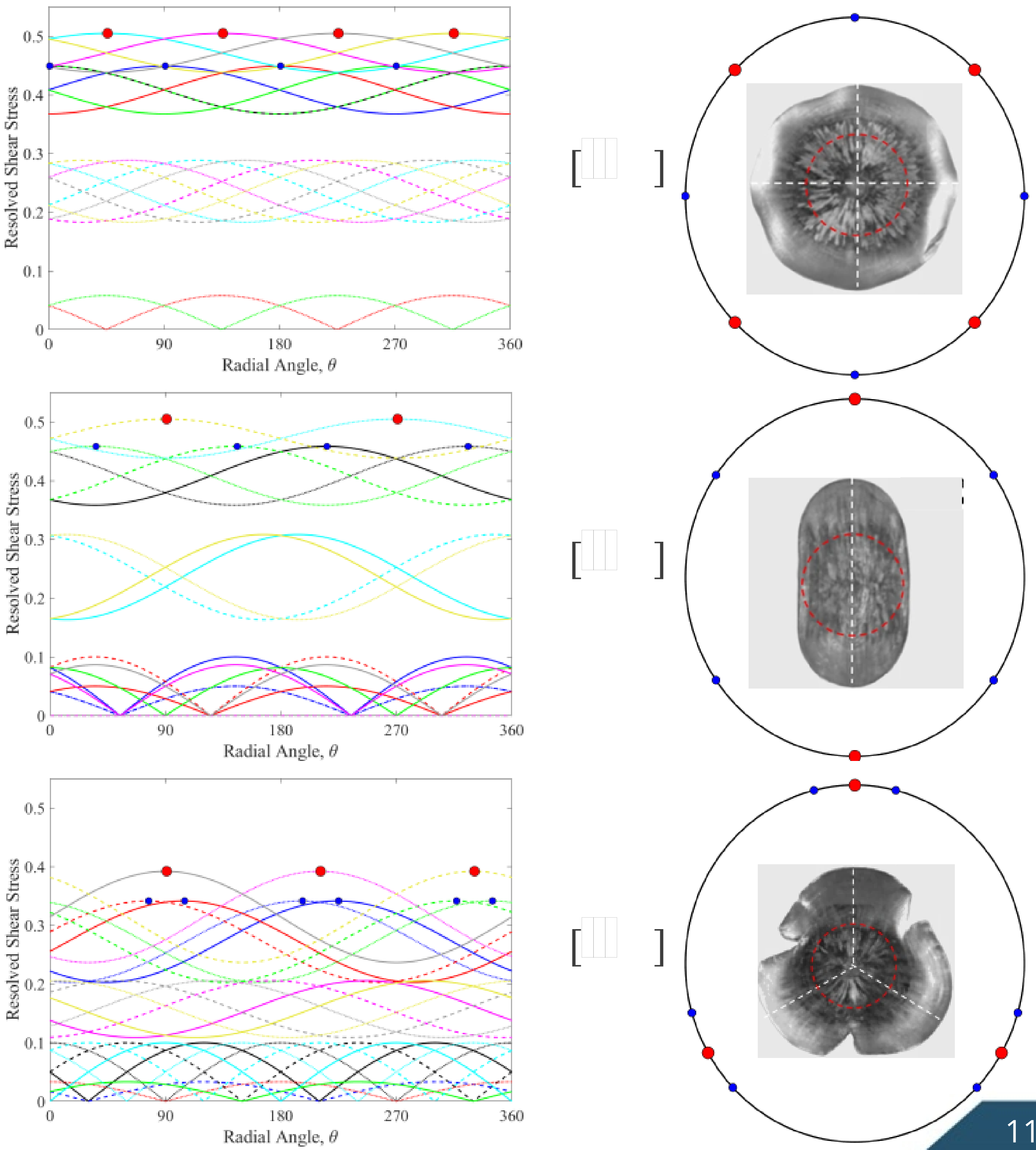


$$\tau_{RSS}(\theta) = \boldsymbol{n} \cdot \boldsymbol{\sigma}(\theta) \cdot \boldsymbol{b}$$

$$\boldsymbol{\sigma}(\theta) = \begin{bmatrix} 0 & 0 & \sigma_{rz} cos\theta \\ 0 & 0 & \sigma_{rz} sin\theta \\ \sigma_{rz}\cos\theta & \sigma_{rz}\sin\theta & \sigma_{zz} \end{bmatrix}$$

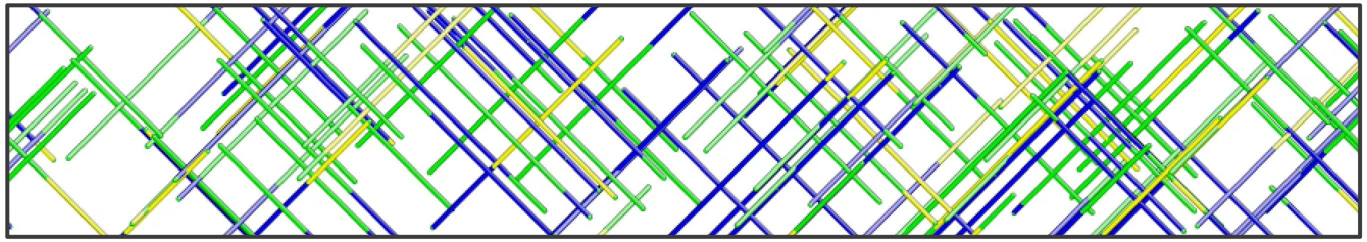
$n=(01\bar{1}), b=[111]$	$n=(011), b=[11\bar{1}]$	$n=(11\bar{2}), b=[111]$	$n=(112), b=[11\bar{1}]$
$n=(\bar{1}01), b=[111]$	$n=(101), b=[11\bar{1}]$	$n=(\bar{2}11), b=[111]$	$n=(2\bar{1}1), b=[11\bar{1}]$
$n=(1\bar{1}0), b=[111]$	$n=(\bar{1}10), b=[11\bar{1}]$	$n=(1\bar{2}1), b=[111]$	$n=(\bar{1}21), b=[11\bar{1}]$
$n=(\bar{1}0\bar{1}), b=[\bar{1}11]$	$n=(10\bar{1}), b=[1\bar{1}1]$	$n=(1\bar{1}2), b=[\bar{1}11]$	$n=(\bar{1}12), b=[1\bar{1}1]$
$n=(0\bar{1}1), b=[\bar{1}11]$	$n=(011), b=[1\bar{1}1]$	$n=(12\bar{1}), b=[\bar{1}11]$	$n=(121), b=[1\bar{1}1]$
$n=(110), b=[\bar{1}11]$	$n=(110), b=[1\bar{1}1]$	$n=(211), b=[\bar{1}11]$	$n=(21\bar{1}), b=[1\bar{1}1]$

- By including shear stress, impact foot shapes can be better predicted
- {112} planes are preferential slip systems with {110} planes being activated next

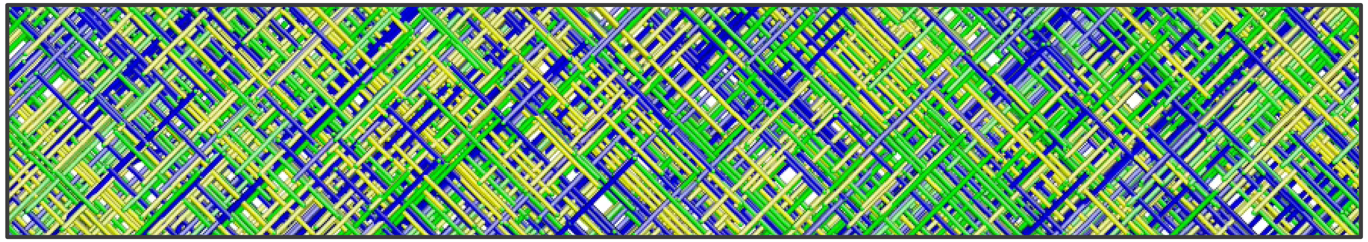


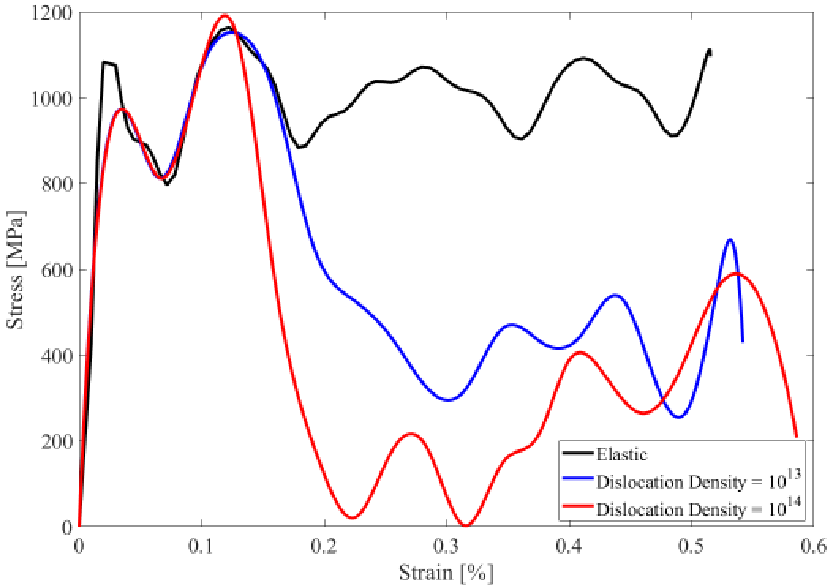
DDEM Results – Initial dislocation density

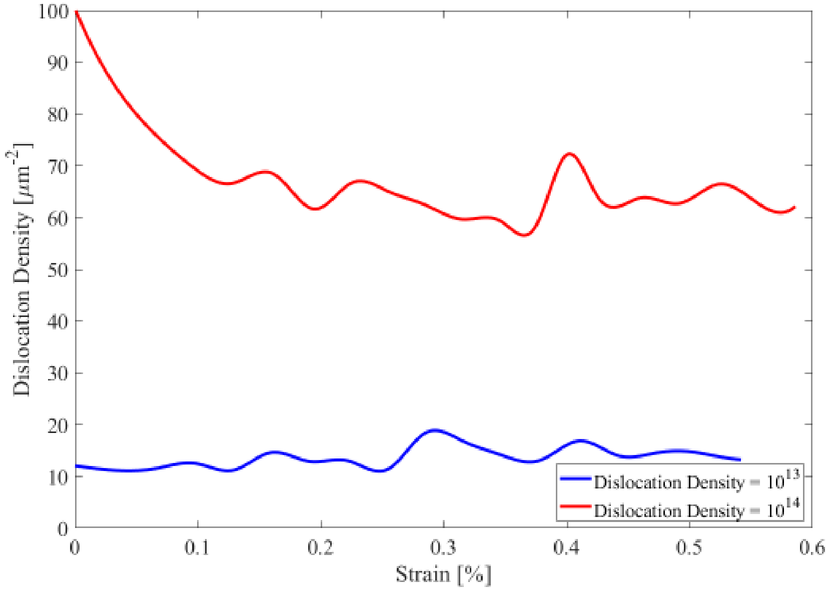
$$\rho_0 = 10^{13}\ m^{-2}$$



$$\rho_0 = 10^{14}\ m^{-2}$$







- Higher dislocation content relaxes stress at the impact foot for the smallest sample size (D = 1.6 μm)

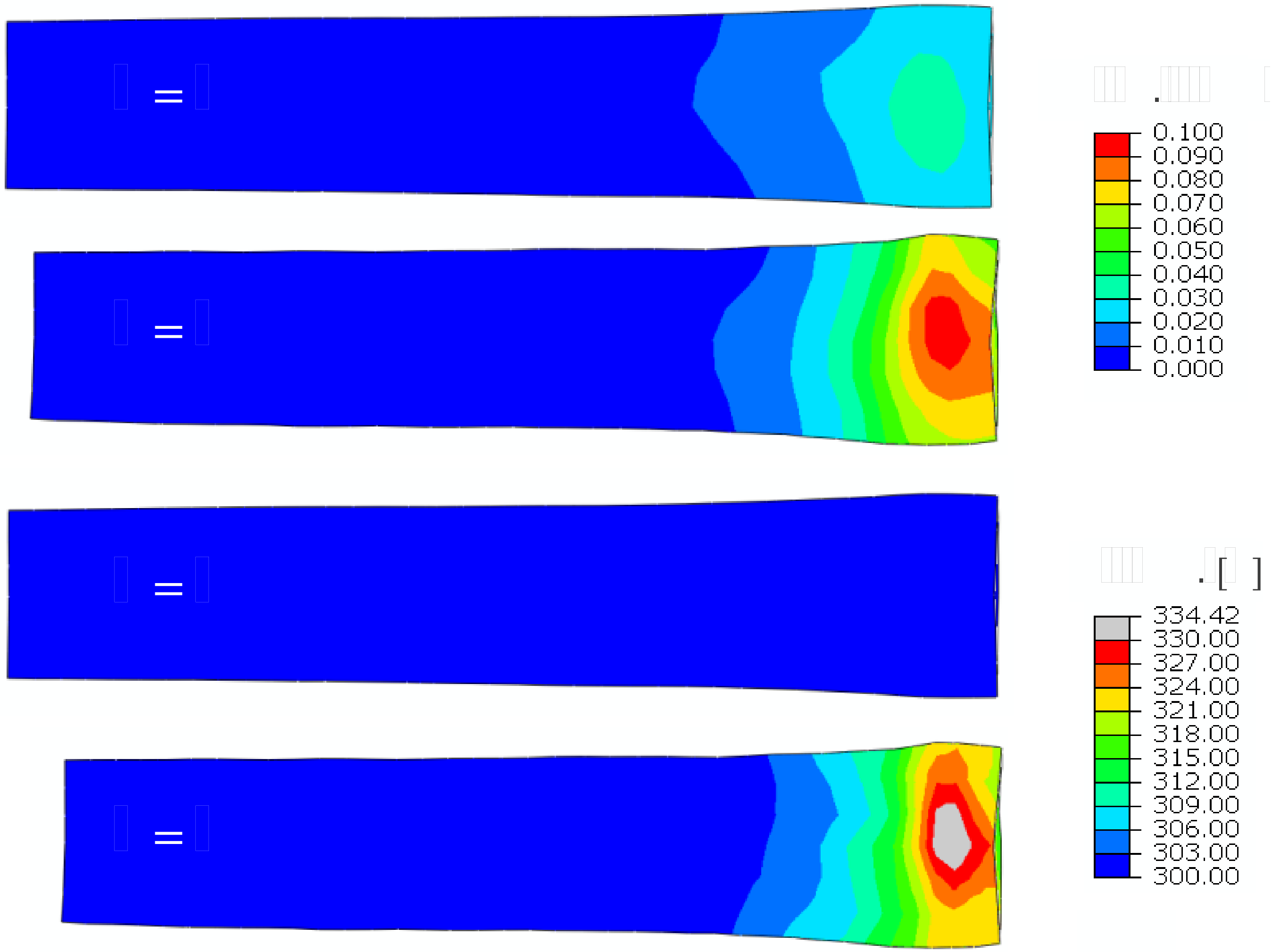
DDEM Results – Temperature

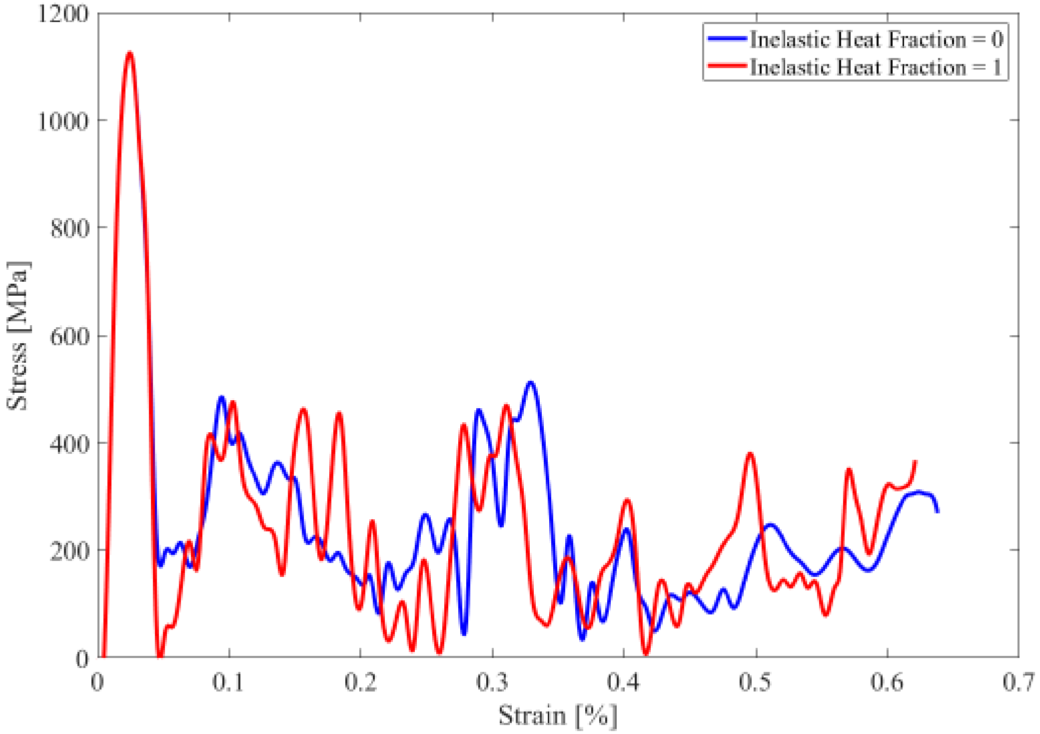
Inelastic heat fraction

$$\Delta T = \eta \frac{(\boldsymbol{\sigma}:\dot{\varepsilon}_p)}{\rho c_p}$$

Plastic dissipation

Material properties





- Temperature does not significantly affect stress-strain response due to the amount of plastic deformation

Summary

- Ta single crystals displayed strong plastic anisotropy during Taylor impact tests
- By concurrently coupling DD and FEM, DDEM can help gain insight on detailed plasticity during Taylor impact
- DDEM can qualitatively predict the anisotropic response observed in experiment along with the effect of initial dislocation density and temperature
- Further work is needed to model larger sample sizes comparable to the experiment

Thank You!