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Integrated Computational Materials Engineering to Establish Process-Structure-Property Relations in Polycrystalline Materials

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Research Engineer, NIA
05/12/2020

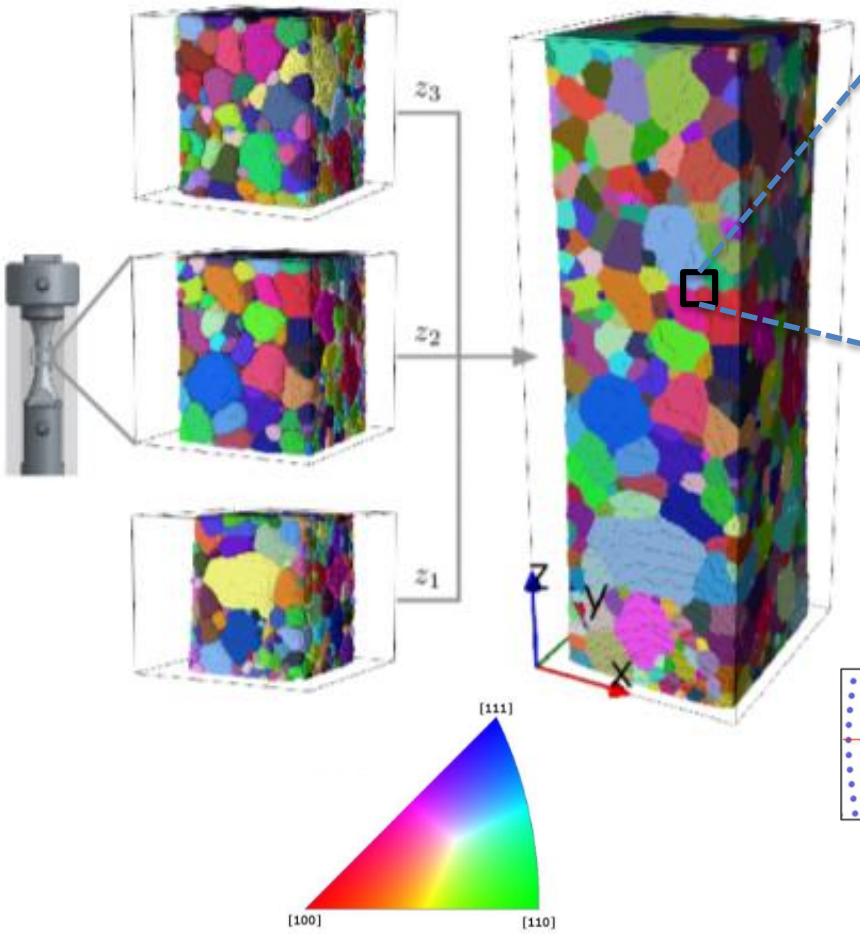
OUTLINE

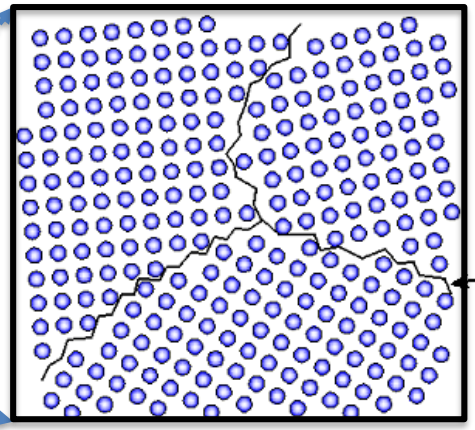
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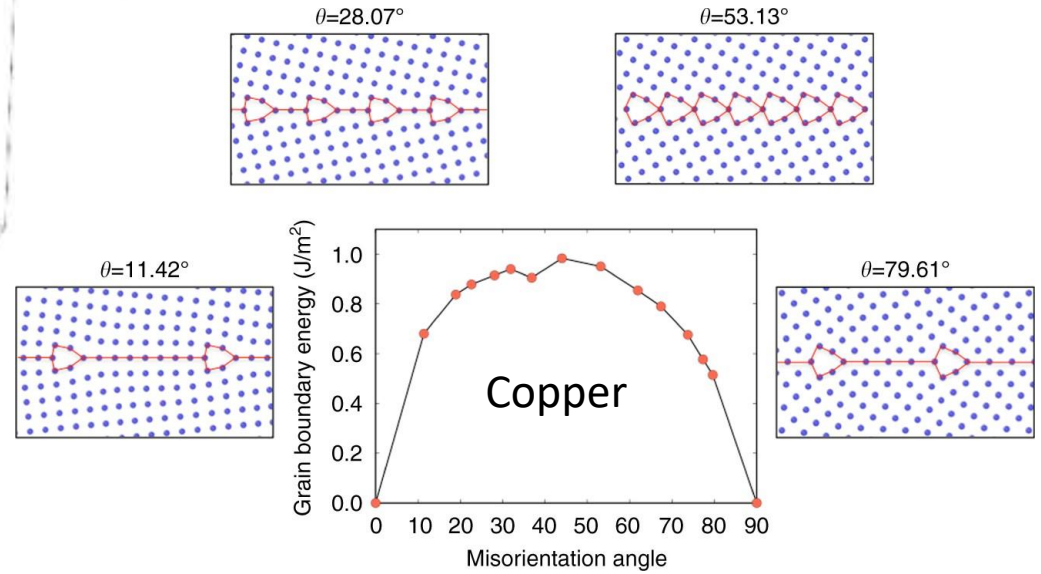
- Background
- Introduction
- Process-Structure-Performance (PSP) Framework
- Strain localization around idealized defects
- Porosity prediction framework

BACKGROUND: POLYCRYSTALLINE MATERIALS

Al-Li alloy







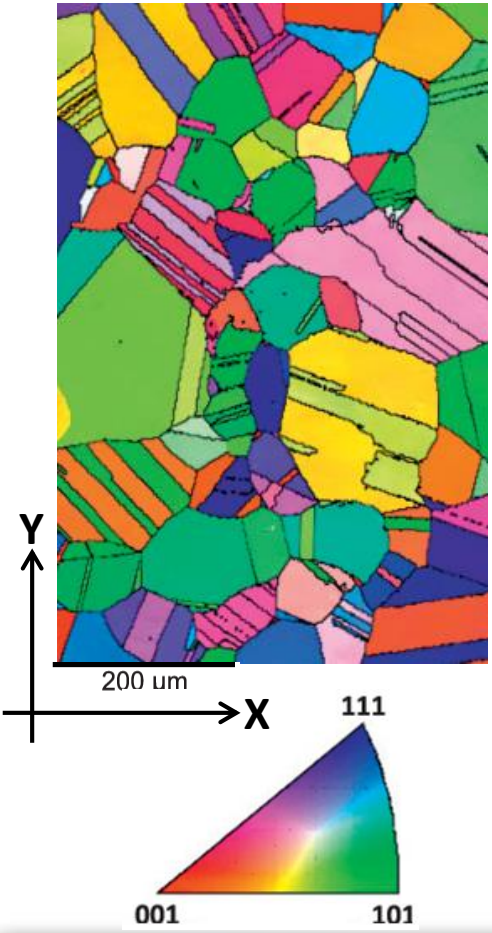
Proudhon et al. (2018) *Materials*
http://www.engineeringarchives.com/les_matsci_surfacedefects.html

Zhu et al. (2018) *Nature Communications*

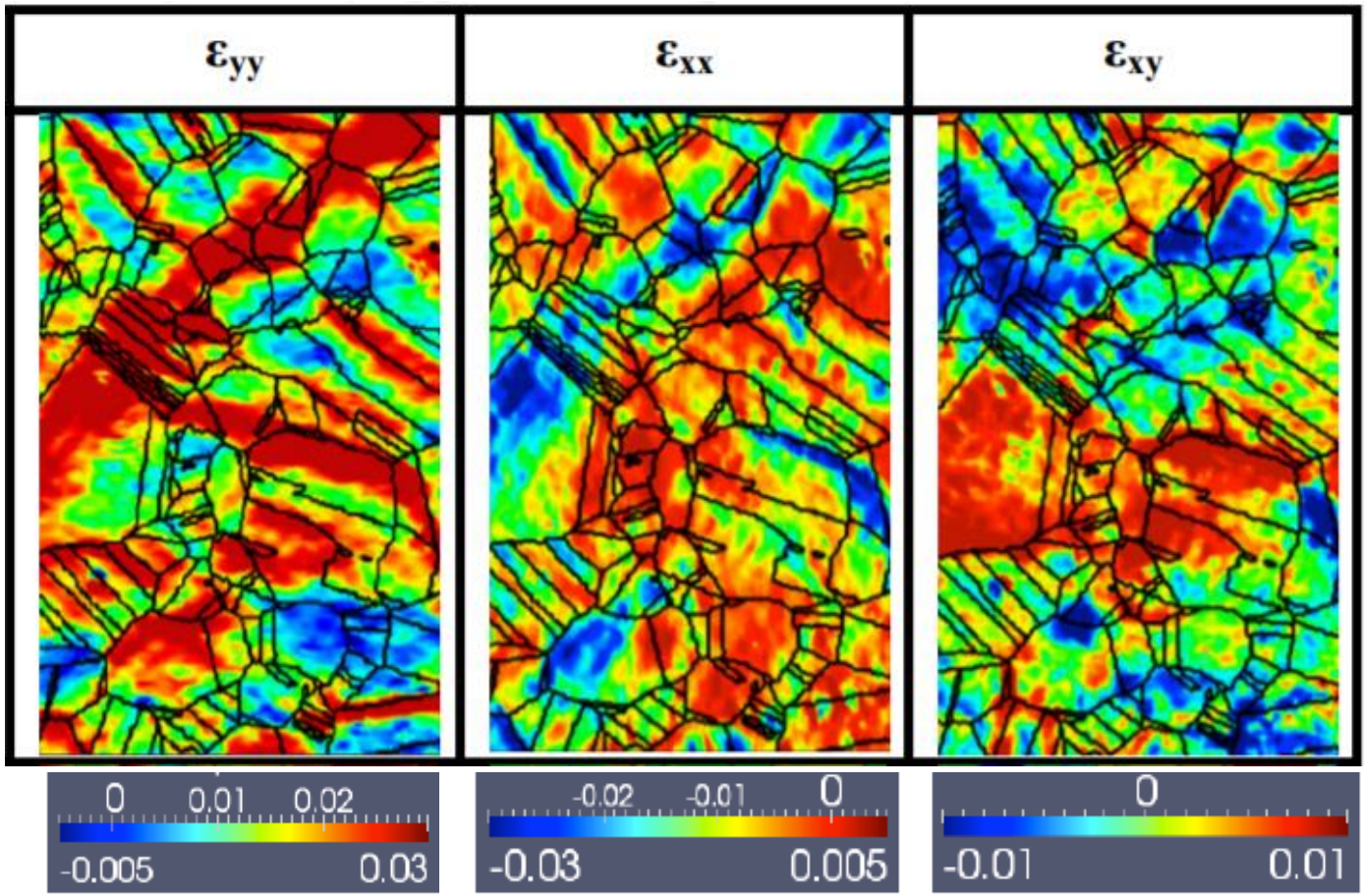
BACKGROUND: STRAIN LOCALIZATION

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Microstructure of a nickel-base alloy

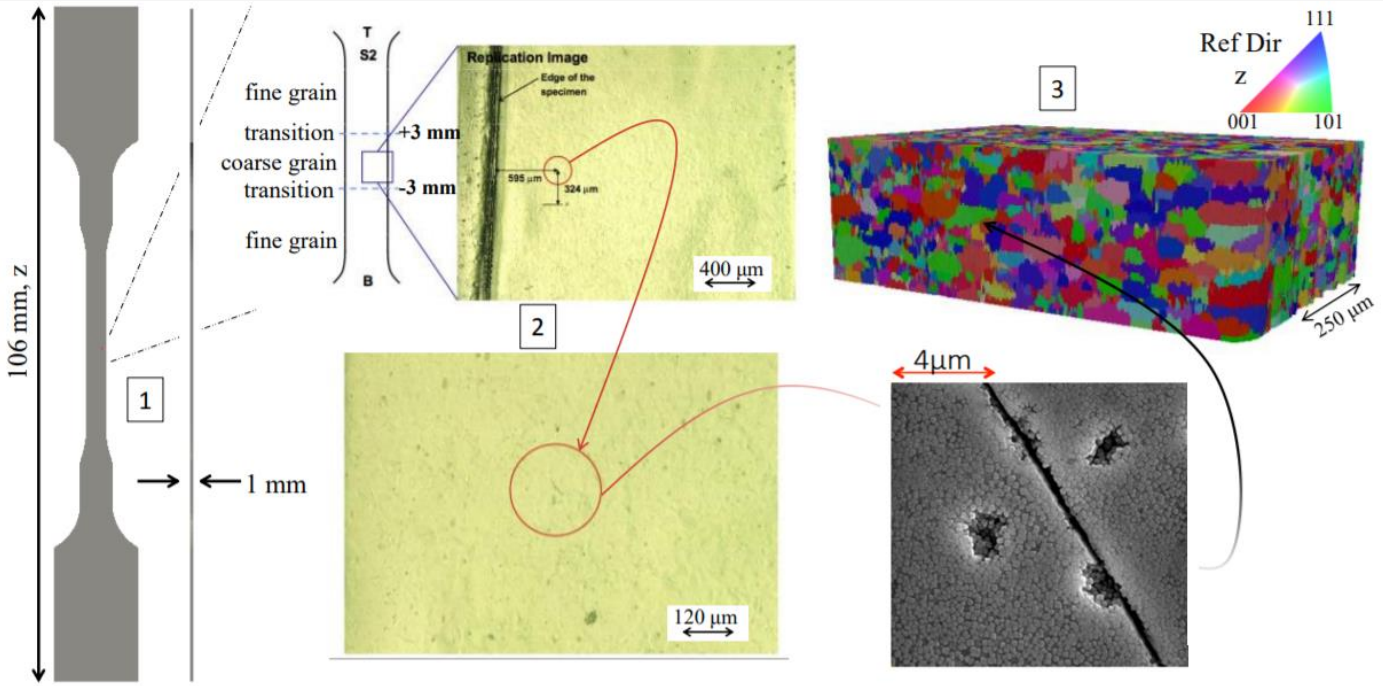


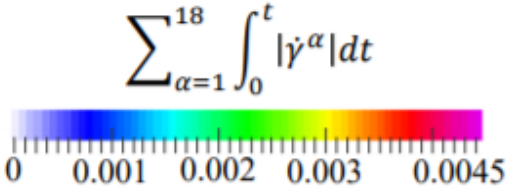
Strain maps obtained from experiments



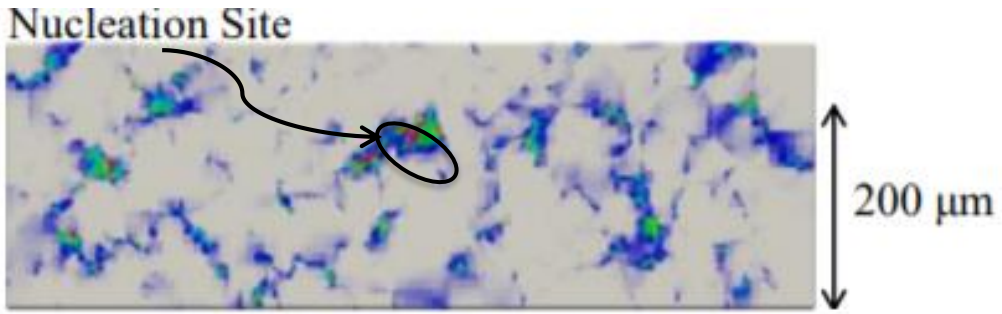
Sangid, Yeratapally, Rovinelli (2014)

BACKGROUND: FATIGUE CRACK INITIATION



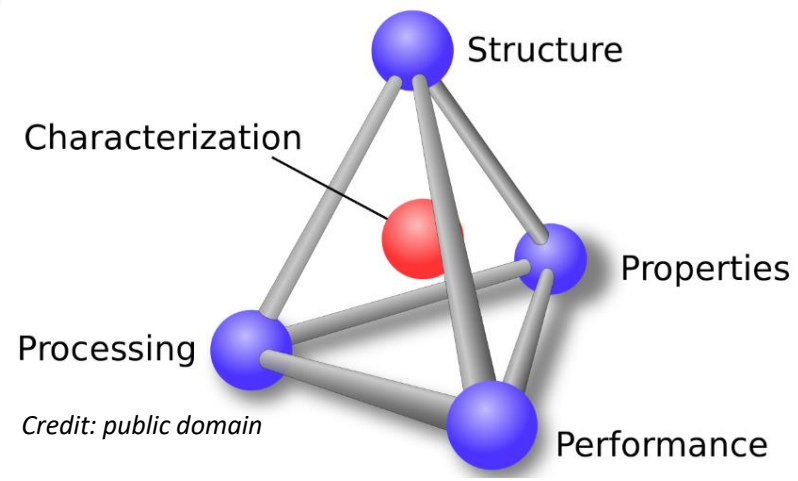


0.20% Applied Strain



Cerrone et al. (2015)

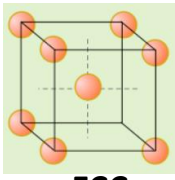
BACKGROUND: PSP RELATIONS



Credit: public domain

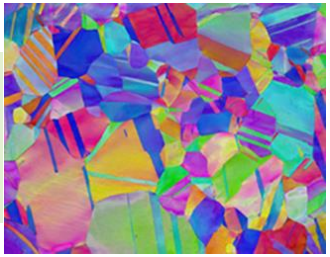


Atomic structure



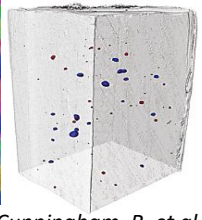
FCC

Microstructure



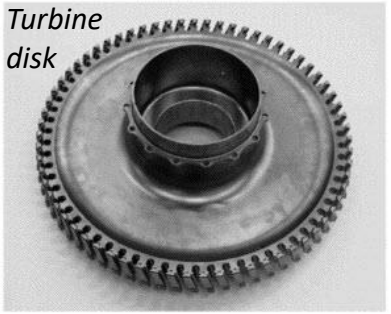
Credit: Hikari

Defect structure

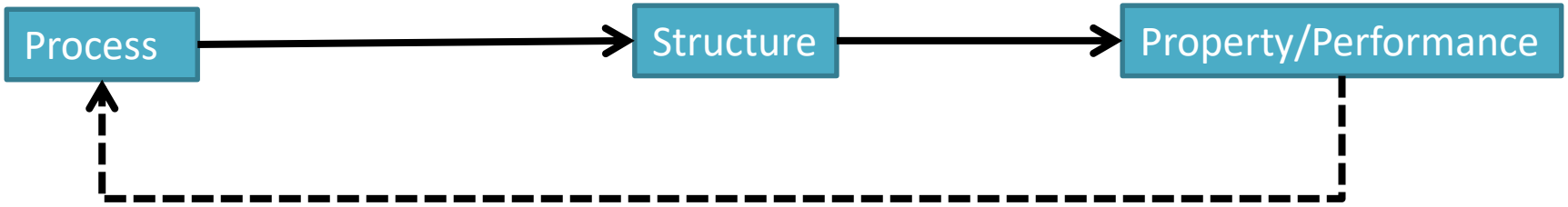


Cunningham, R. et al.

Turbine disk



Credit: public domain



BACKGROUND

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Microstructure ✓

Heterogeneous strain localization ✓

Fatigue crack initiation ✓

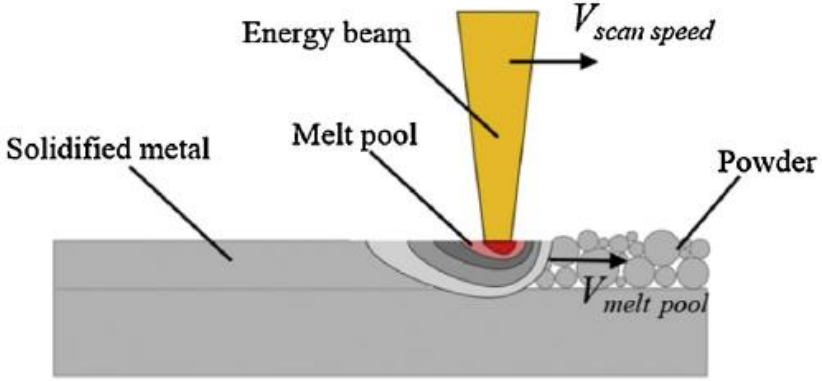
PSP linkage ✓

OUTLINE

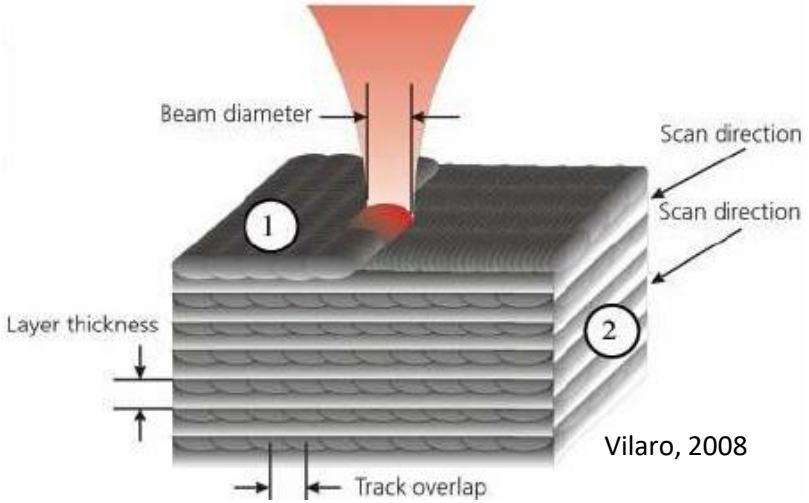
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INTRODUCTION: SELECTIVE LASER MELTING

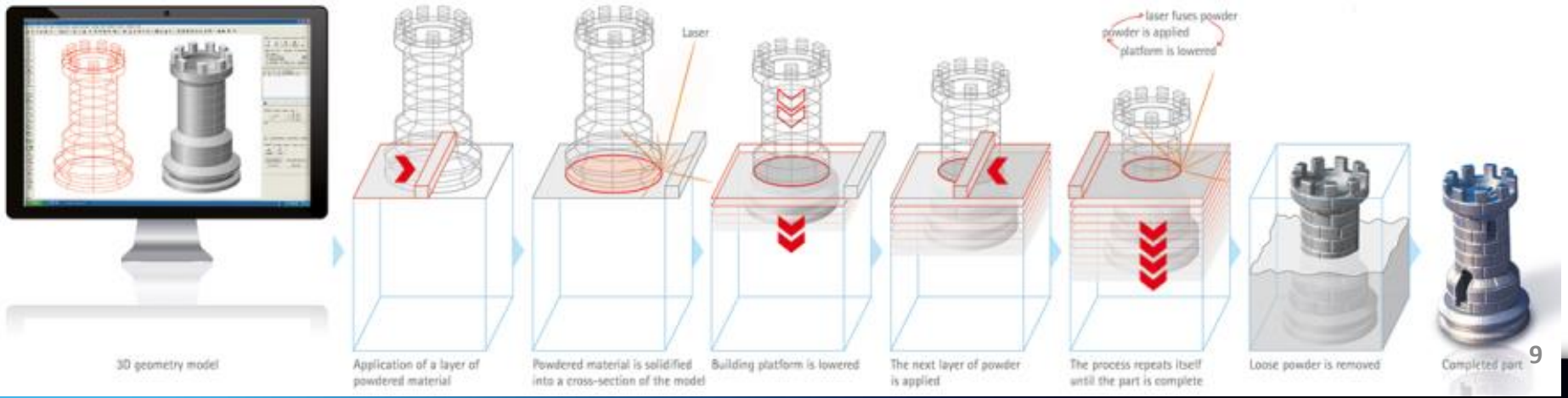
Selective Laser Melting (SLM): An additive manufacturing (AM) technique that uses a high-power density laser to melt and fuse metallic powders together into a 3D component



H. Gong et al. / Additive Manufacturing 1–4 (2014) 87–98



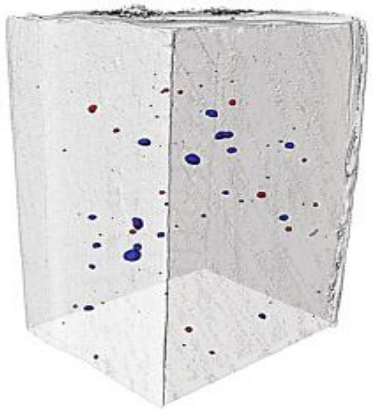
Vilaro, 2008



INTRODUCTION: DEFECTS IN SLM PROCESS

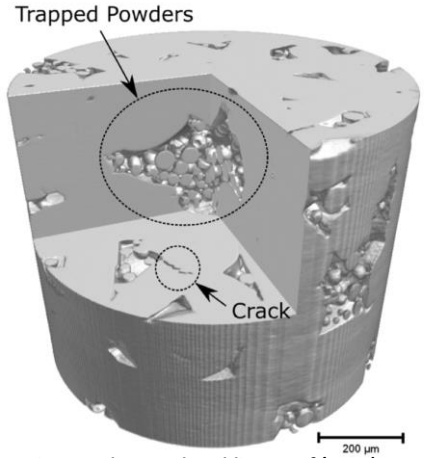
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Keyhole porosity



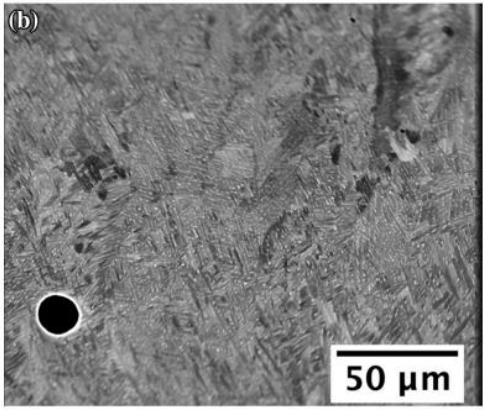
Cunningham, R. et al. JOM, Vol. 69, No. 3, 2017

Lack of fusion (LoF) porosity



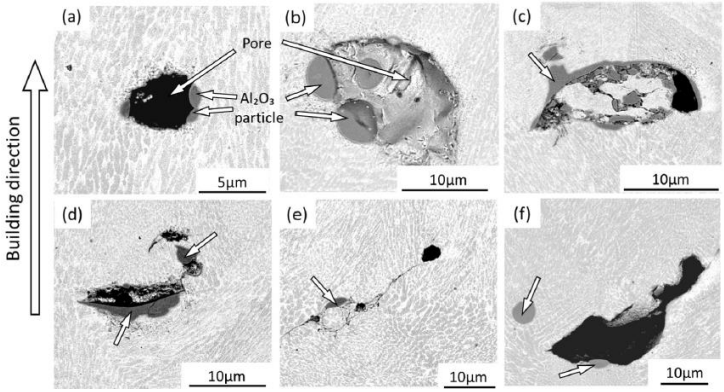
Kim, Moylan, et al., Addit Manuf (2017)

Entrapped gas (EG) porosity



JOM, Vol. 68, No. 3, 2016 DOI: 10.1007/s11837-015-1802-0

Oxide induced porosity



Tang et al. Int. J. Fatigue, Vol. 94, 2017, pp. 192-201

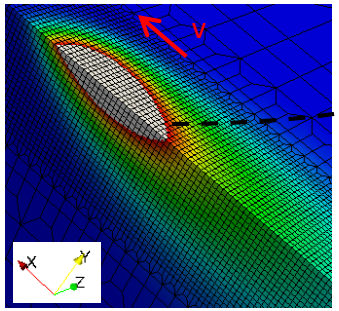
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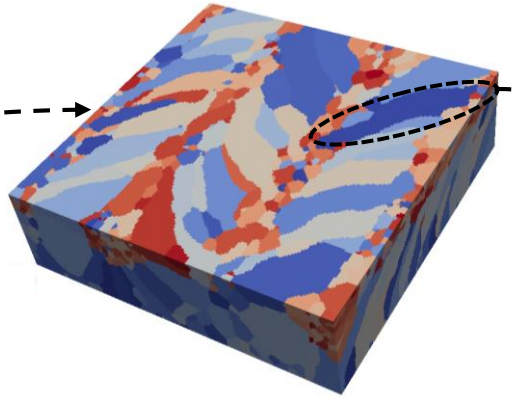
PSP FRAMEWORK FOR SLM PROCESS

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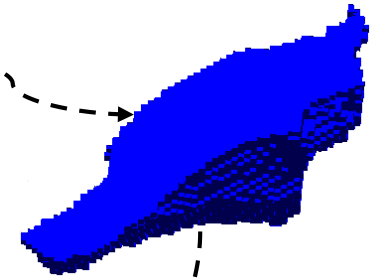
Finite Element Thermal Analysis



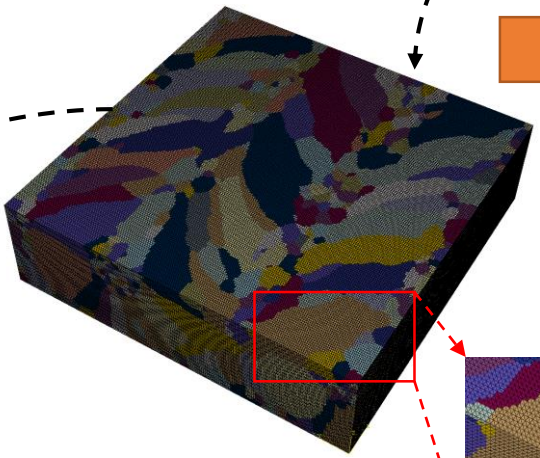
AM process simulation SPPARKS[1]

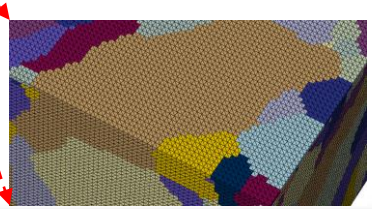


Use Output from SPPARKS and generate .stl files of grains using DREAM. 3D[2]



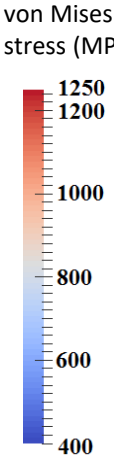
Gmsh[3]





Use ScIFEN[4] to solve for heterogeneous stress/strain fields





Yeratapally et al. (2020)

[1]SPPARKS: spparks.sandia.gov [2]DREAM.3D: dream3d.bluequartz.net [3]Gmsh: gmsh.info [4]ScIFEN: https://software.nasa.gov/software/LAR-18720-1

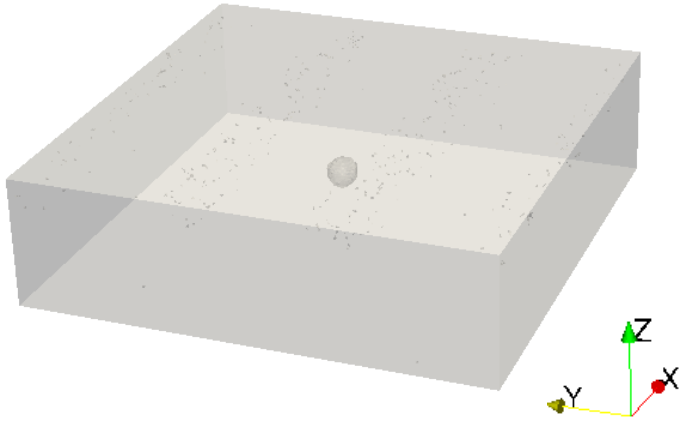
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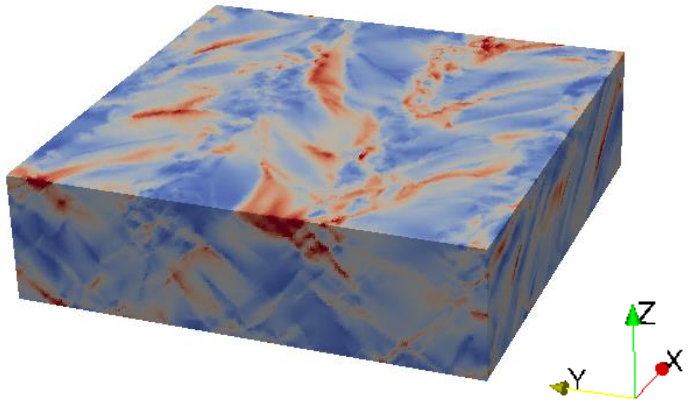
STRAIN LOCALIZATION NEAR IDEALIZED KEYHOLE PORES

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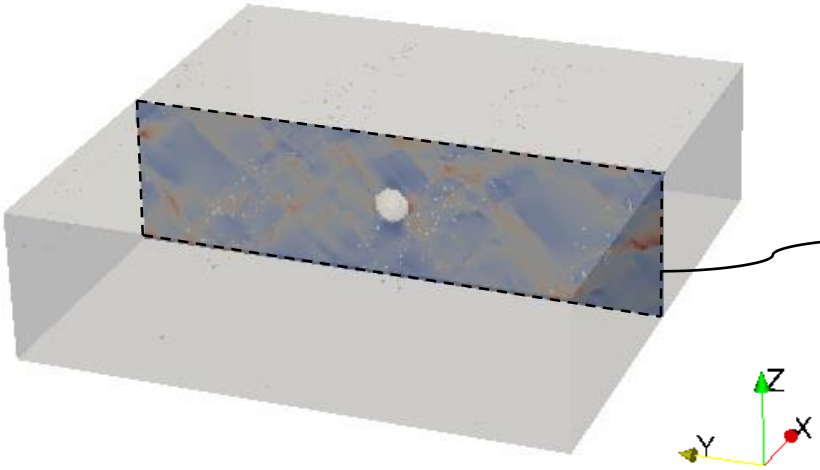
Microstructure volume showing the location of pore



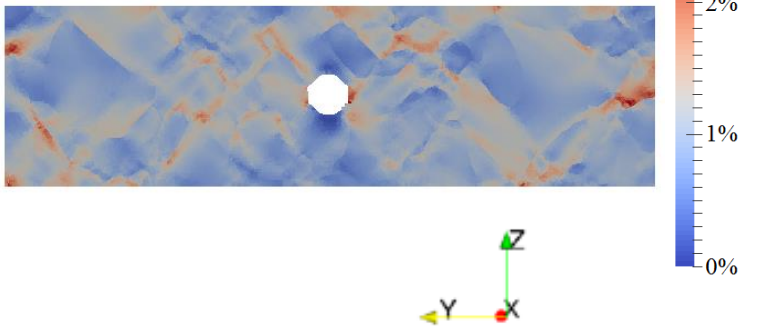
Heterogeneous strain field generated in the microstructure



Strain field on a plane passing through the pore



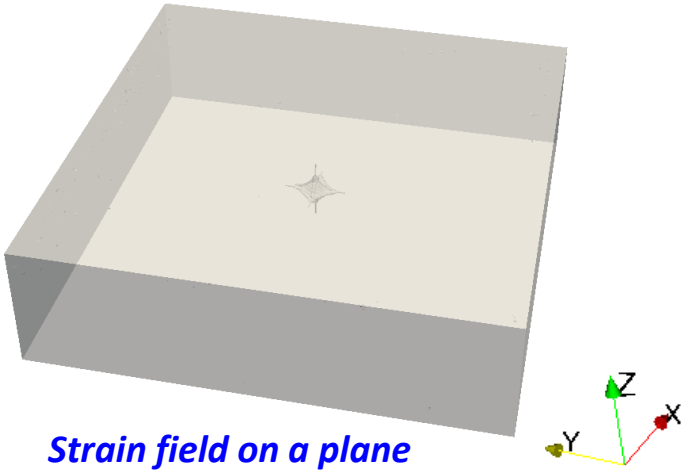
Slice view of strain field around the pore



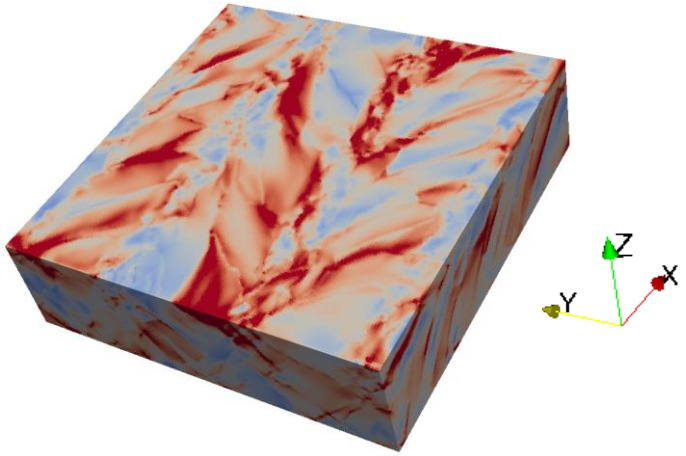
STRAIN LOCALIZATION NEAR IDEALIZED LoF PORES

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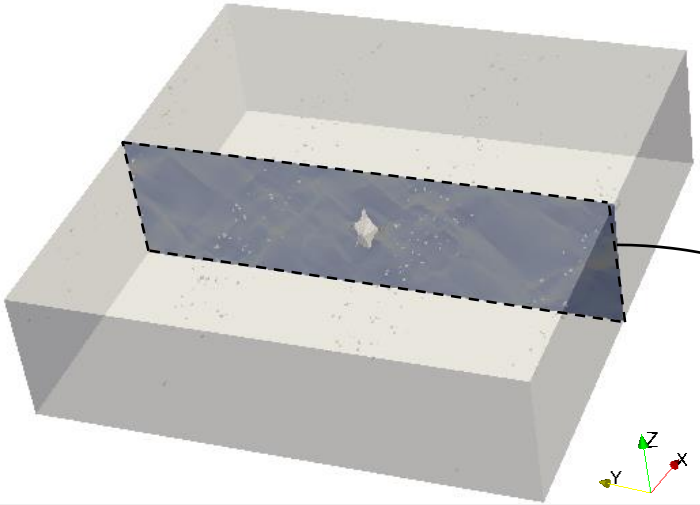
Microstructure volume showing the location of pore



Heterogeneous strain field generated in the microstructure



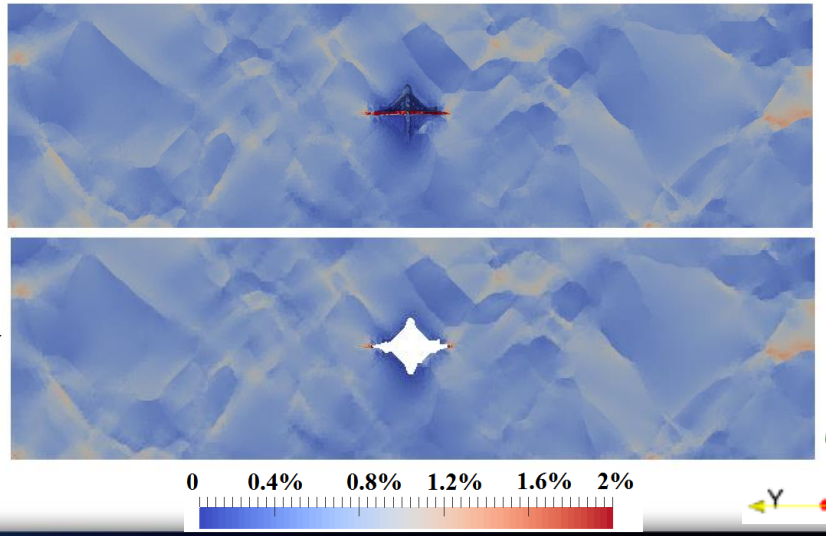
Strain field on a plane passing through the pore



Clip view

Slice view

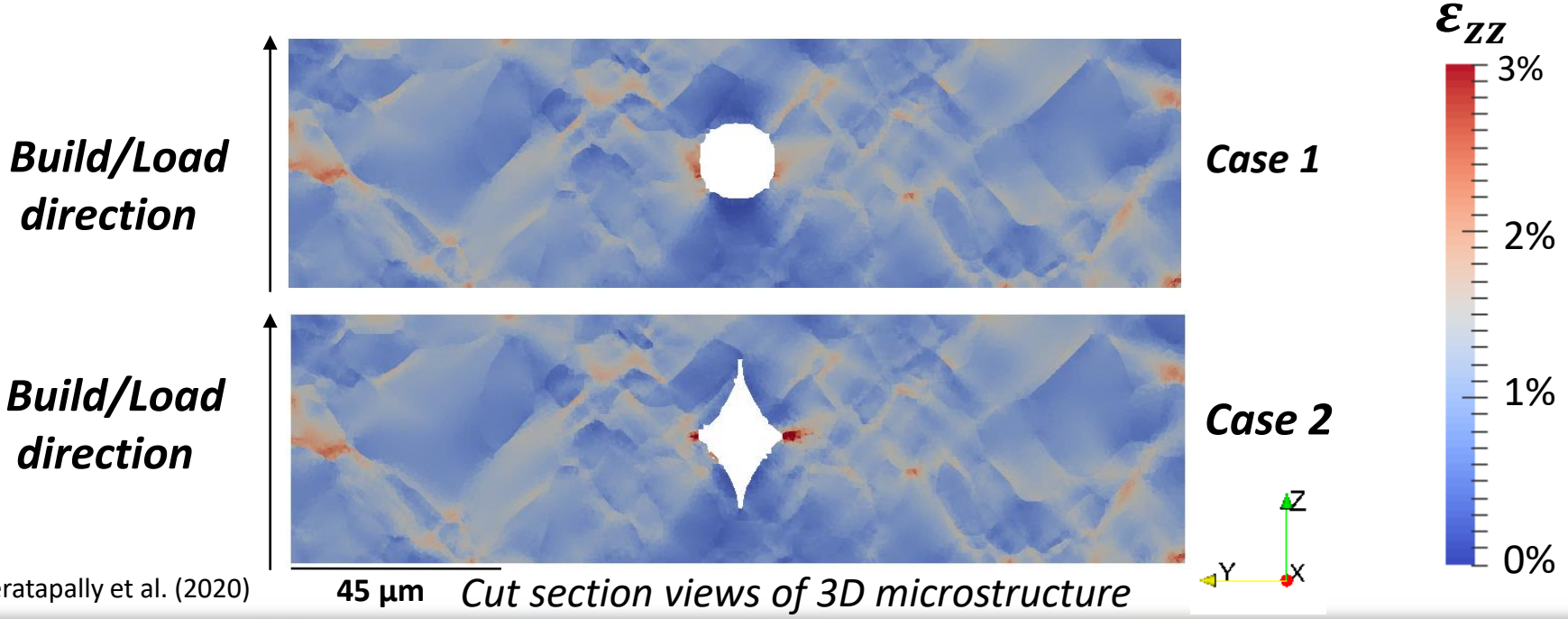
Strain field around the pore



ε_{zz} (strain component in loading direction)

CASE STUDY: EFFECT-OF-DEFECT MORPHOLOGY

- Material: IN 718
- LoF (super-ellipsoids) vs. keyhole (spherical) pores
- Surrounding microstructure is the same in both cases
- Pore volume fraction is the same in both cases
- Global strain applied: 1%
- Observation: Strain localization is intense for LoF pore with sharp corners compared to the idealized keyhole pore of the same volume

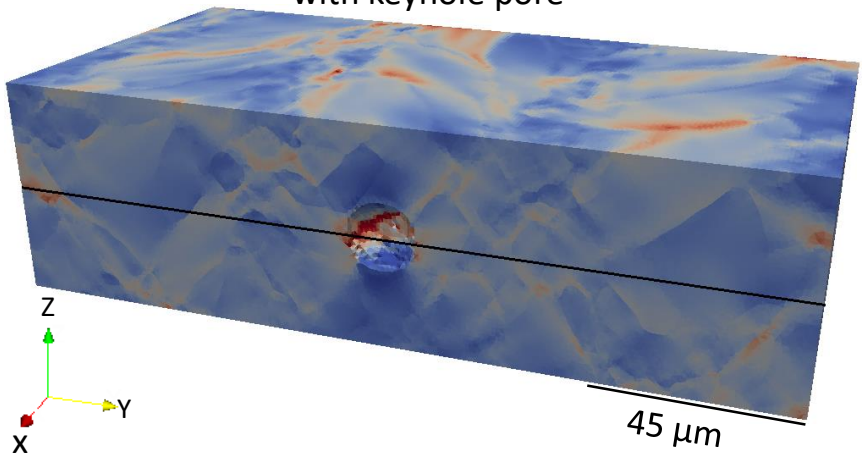


Yeratapally et al. (2020)

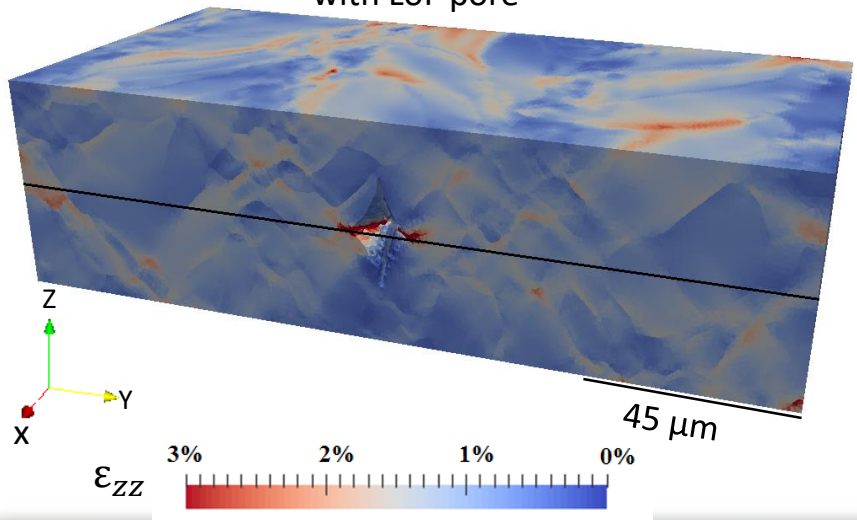
Cut section views of 3D microstructure

CASE STUDY: EFFECT-OF-DEFECT MORPHOLOGY

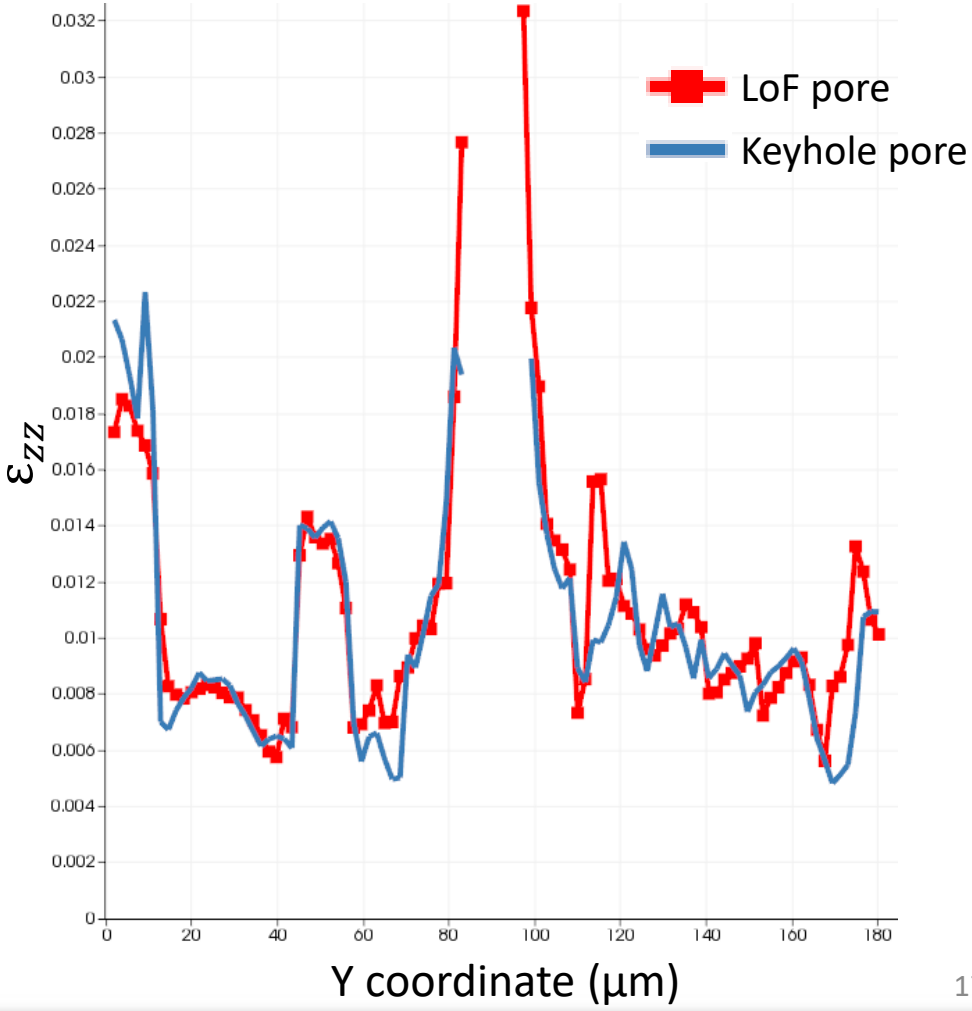
Cut section view of the 3D microstructure with keyhole pore



Cut section view of the 3D microstructure with LoF pore



Strain component in the loading direction (ε_{zz}) along a trace line (in black) passing through the middle of the pore



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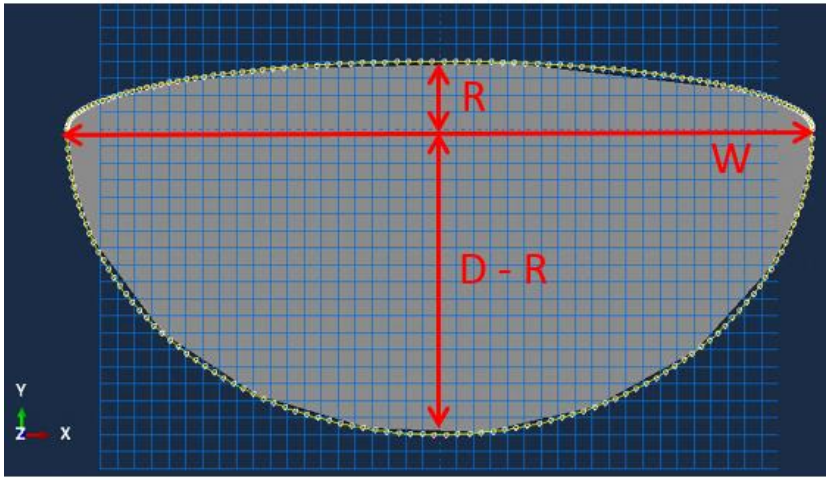
IDEALIZATION OF A SCAN TRACK

Rosenthal Equation:

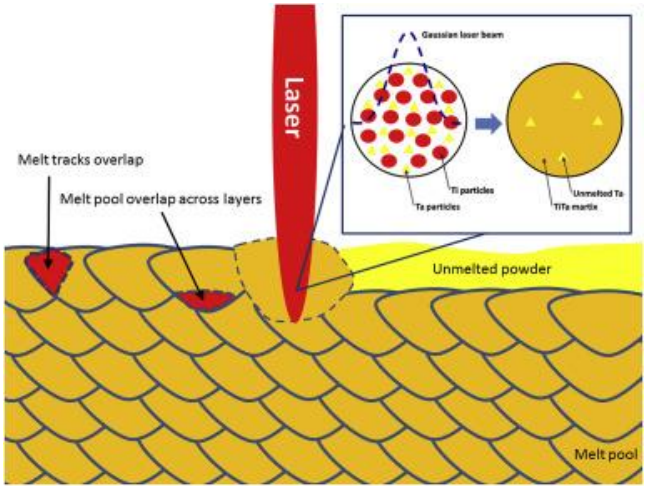
$$Q = \pi k(T_f - T_o)W + e\pi\rho C(T_f - T_o)VW^2/8$$

- Q Absorbed Power
- k Thermal Conductivity
- C Heat Capacity
- ρ Density
- T_f Melting Point
- T_o Ambient Temp

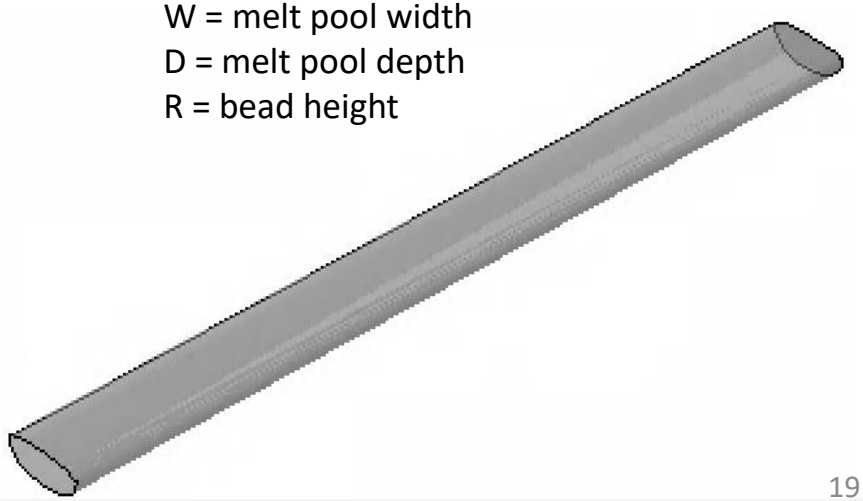
Cross-section of the melt pool



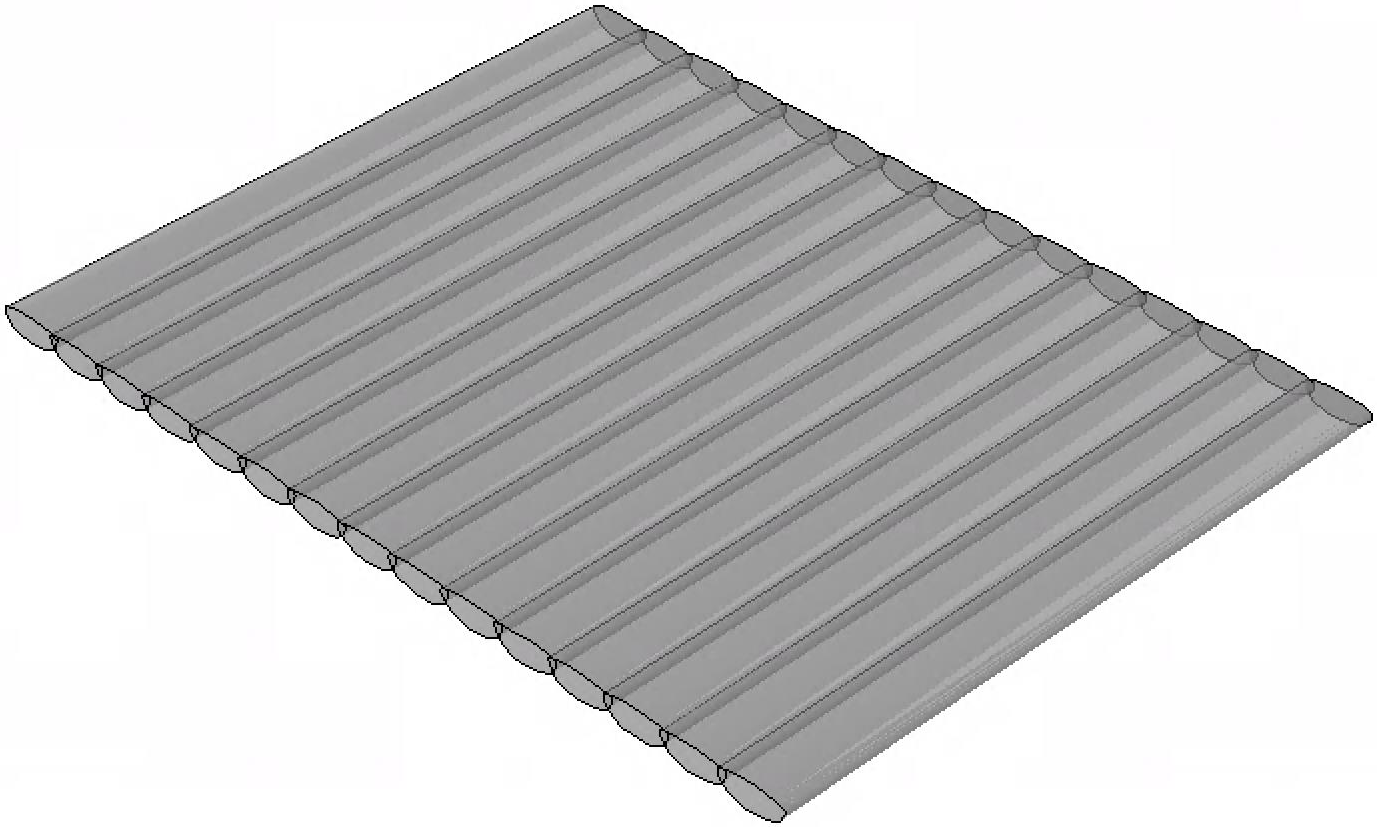
W = melt pool width
D = melt pool depth
R = bead height



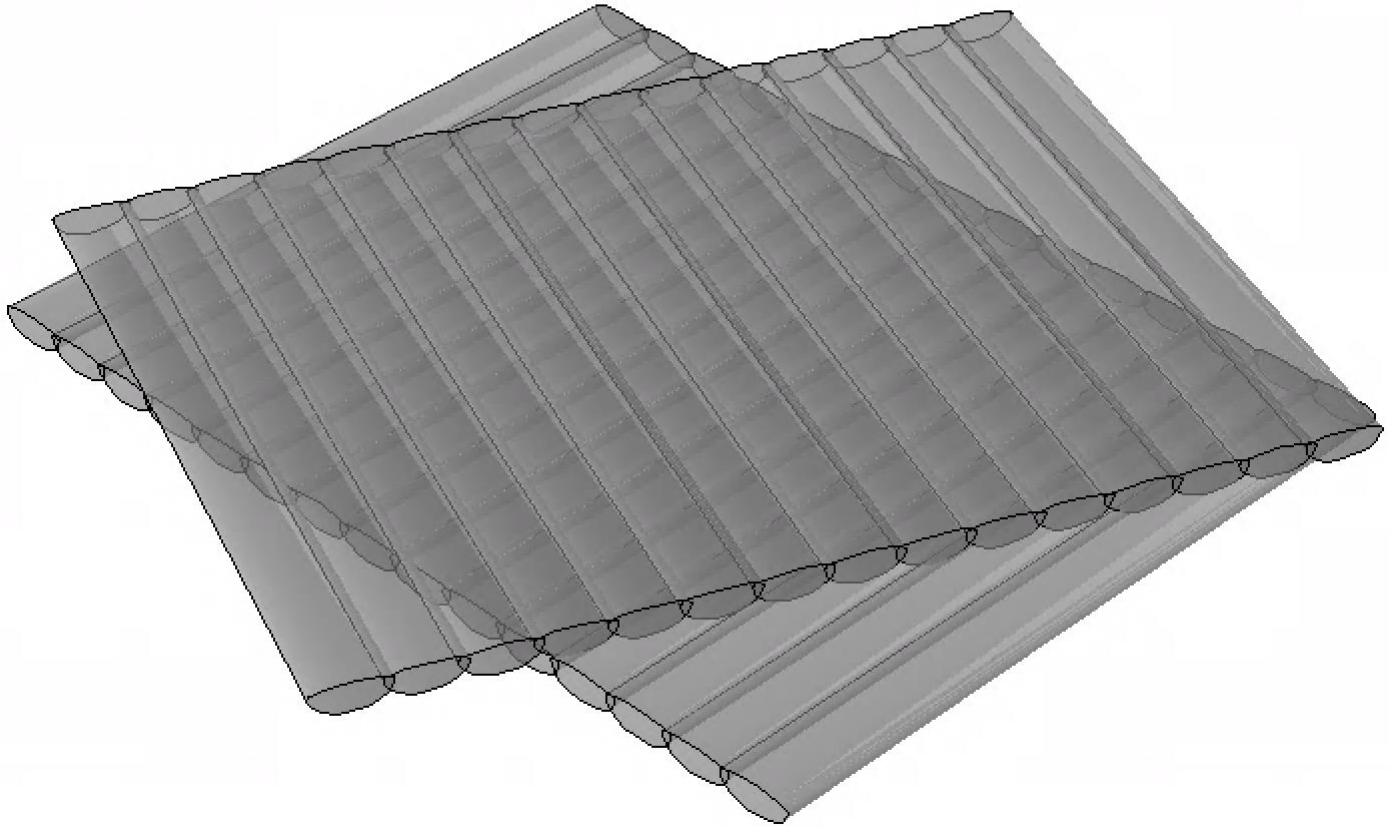
Sing et al. (2016)



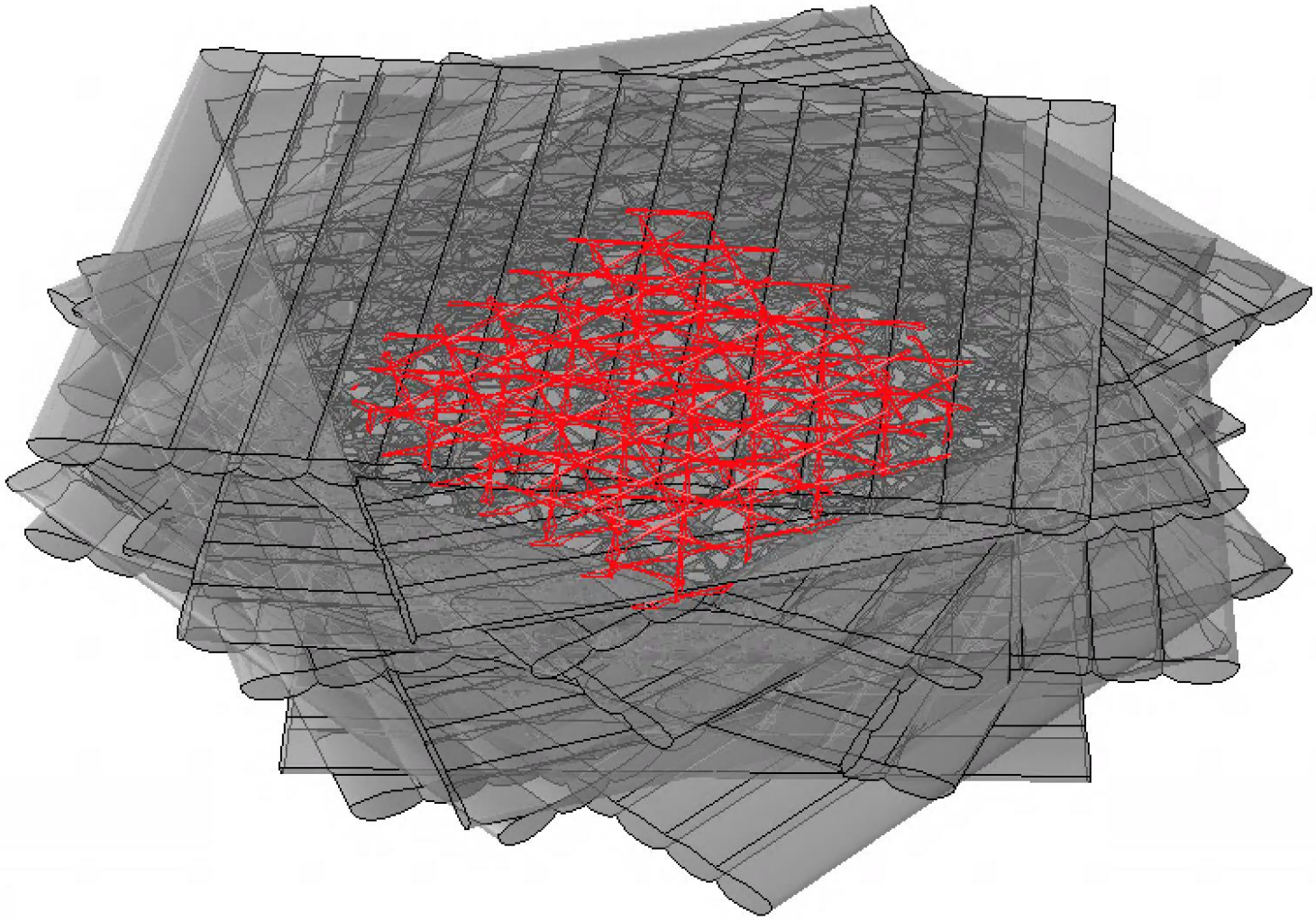
IDEALIZATION OF A SCAN LAYER



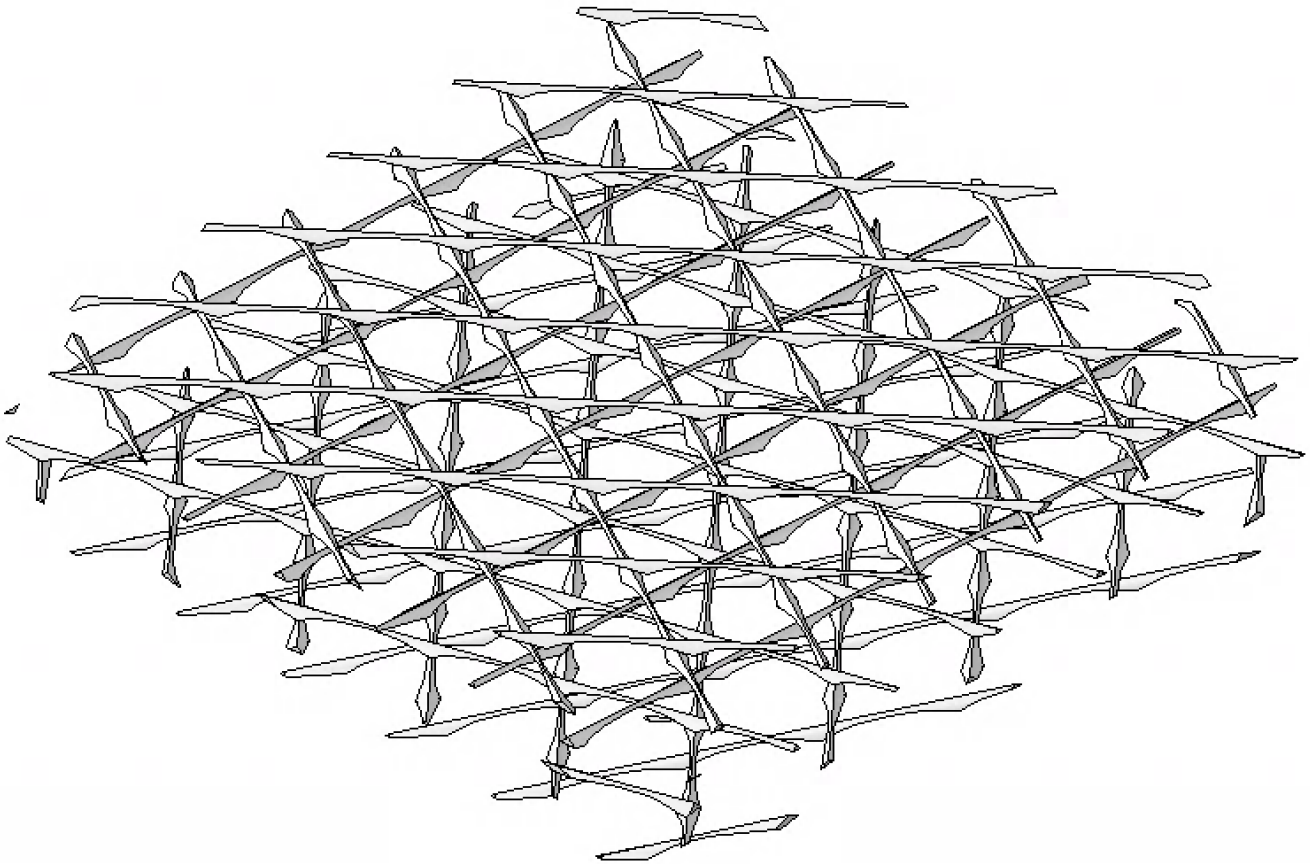
TWO SCAN LAYERS



UNMELTED REGIONS IN BUILD

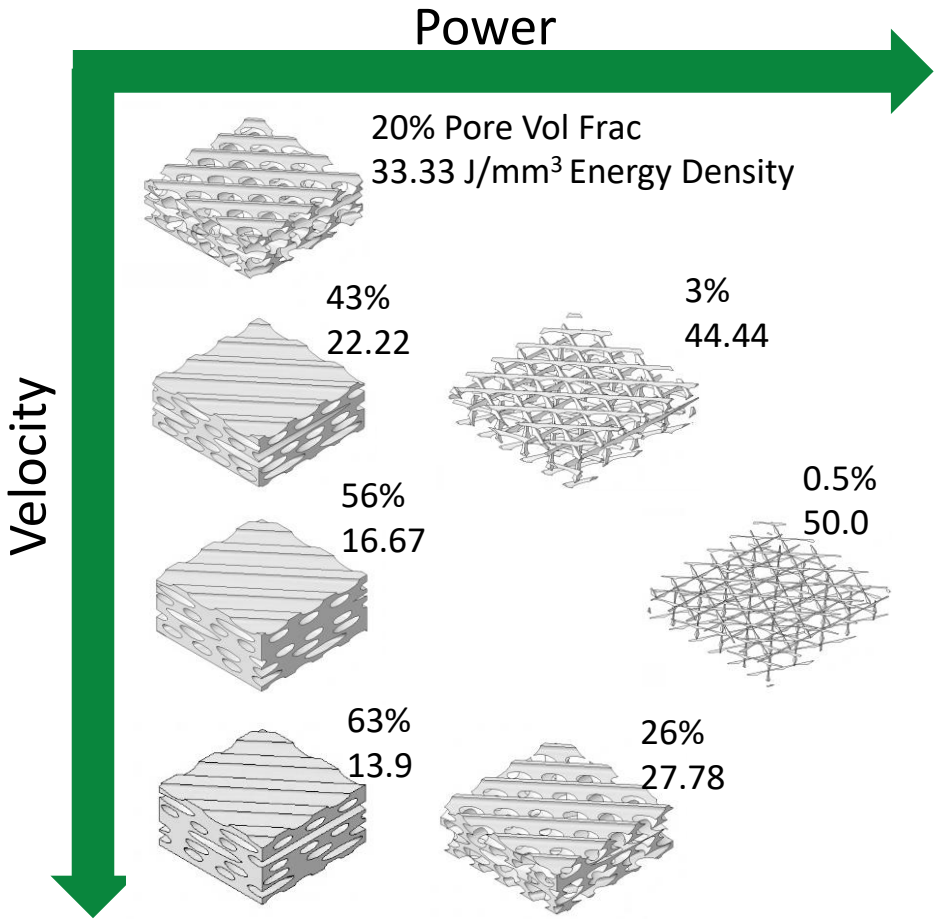


LoF PORE MORPHOLOGIES

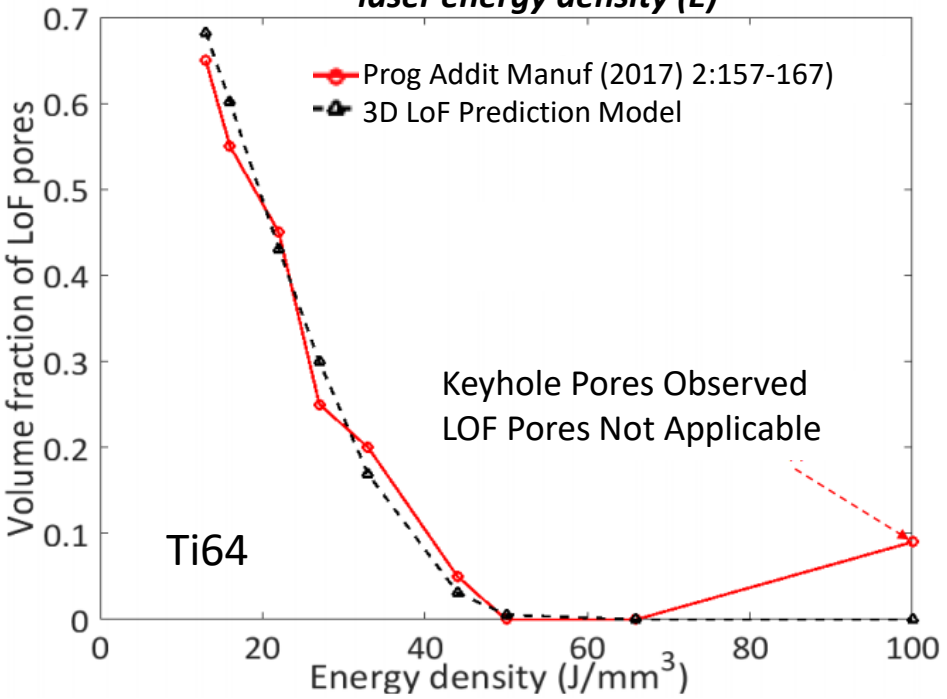


PARTIAL VALIDATION

R = 10 µm L = 30 µm H = 100 µm D/W = 0.4



Variation of volume fraction of LoF porosity with laser energy density (E)

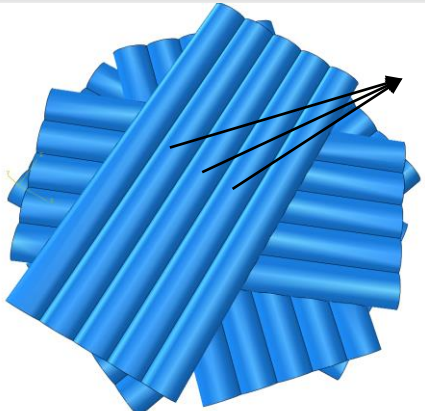


$$E = \frac{P}{VHL}$$

OVERVIEW OF POROSITY PREDICTION FRAMEWORK

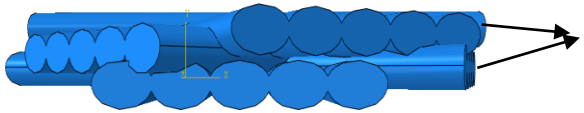
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Top view

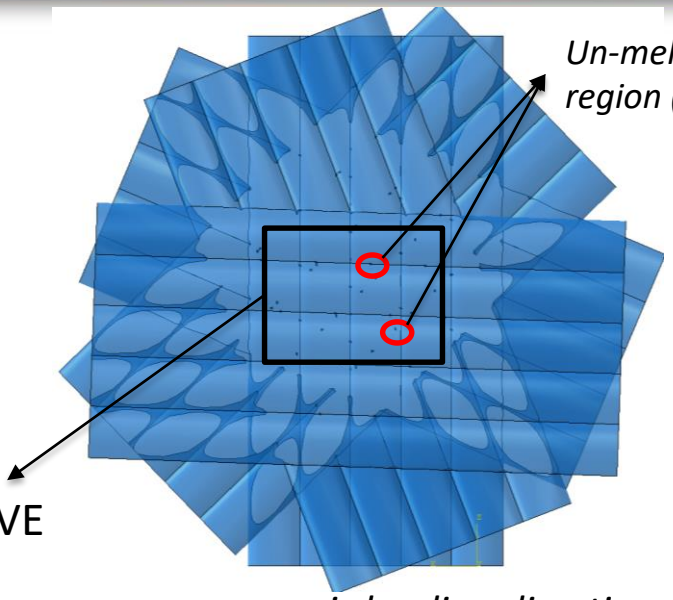


Scan tracks (67 degree hatch rotation)

Side view

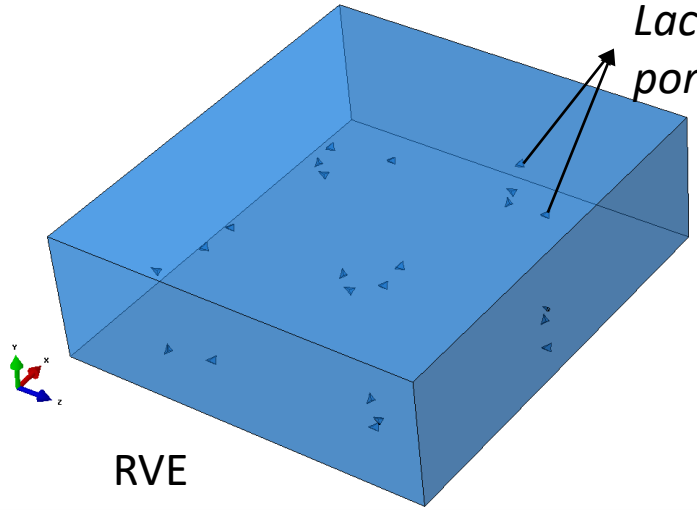


Deposition layers



Un-melted region (Pores)

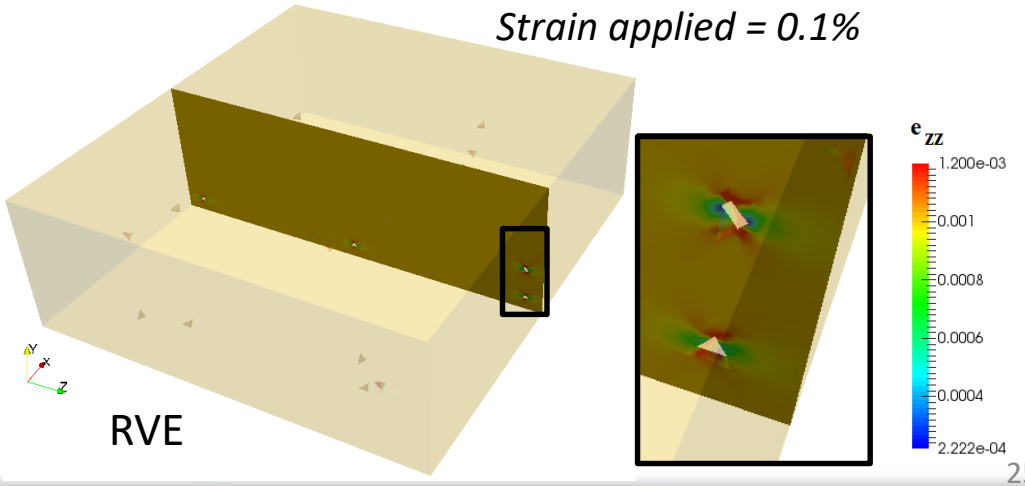
RVE



Lack-of-fusion pores

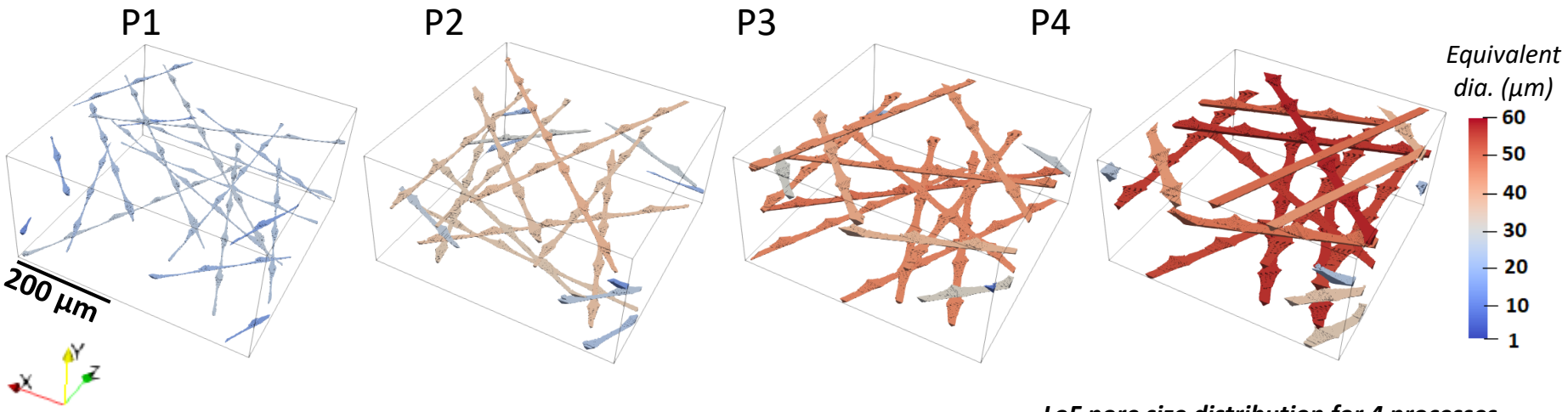
RVE

zz is loading direction
Strain applied = 0.1%



RVE

CHARACTERIZATION OF DEFECTS

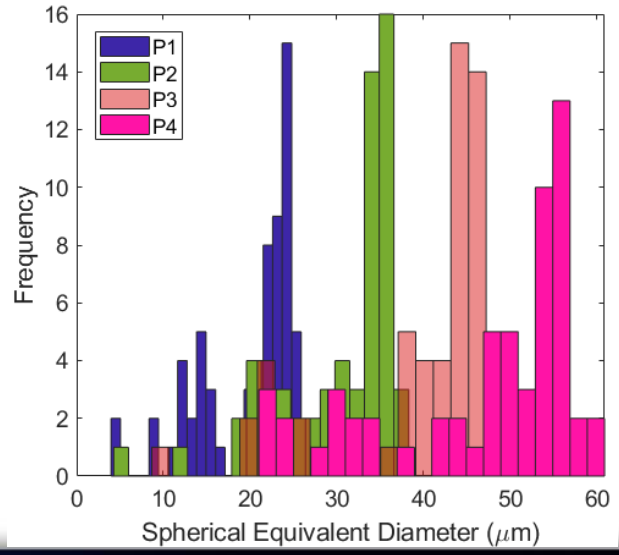


Process	P (W)	V (m/s)	E (J/mm^3)	Equ. dia (μm)
P1	150	1	50	19.75
P2	140	1	46.67	30.51
P3	100	0.75	44.44	38.96
P4	150	1.25	31.57	46.93

$$E = \frac{P}{VHL}$$

H = 100 μm
L = 30 μm
Θ = 67°

LoF pore size distribution for 4 processes (P1,P2,P3,P4)



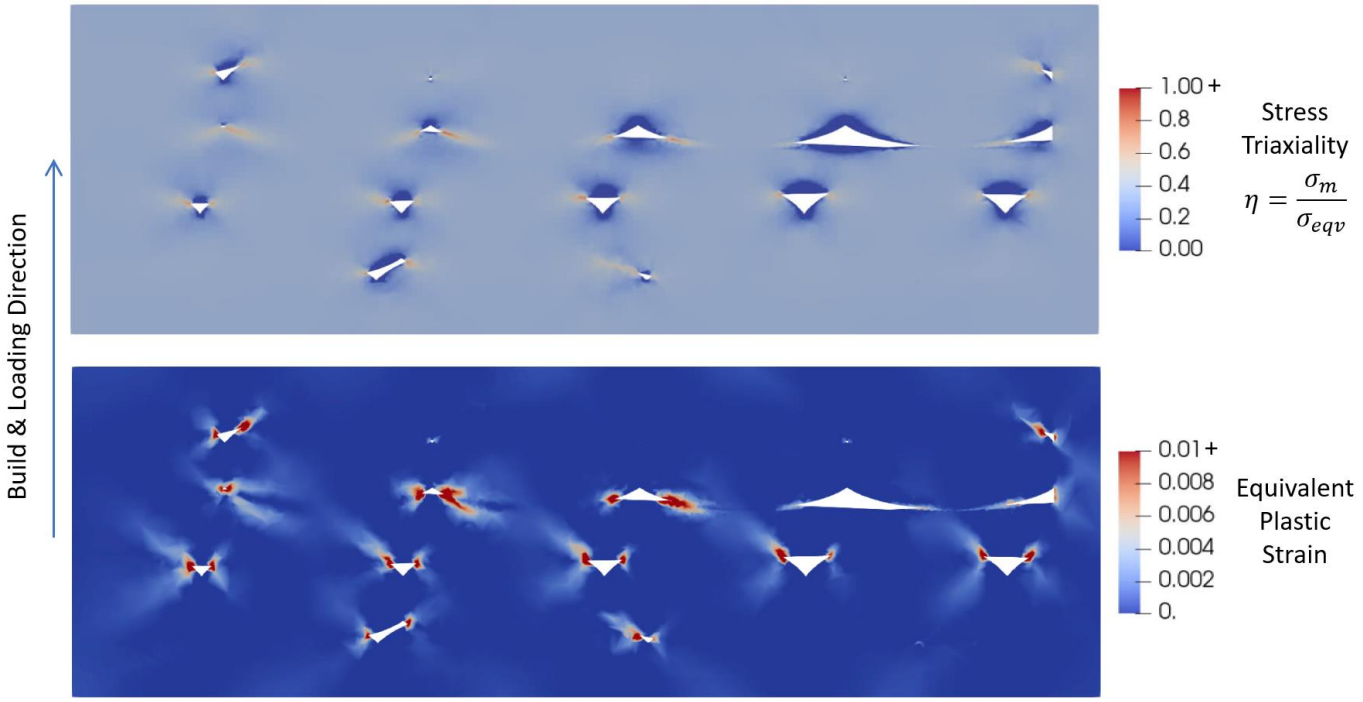
STRAIN ACCUMULATION

Modeling details:

i) Solve for defect distribution using a porosity prediction model

ii) Use isotropic elastic-plastic properties on the RVE to calculate fatigue crack driving forces in a finite element driver.

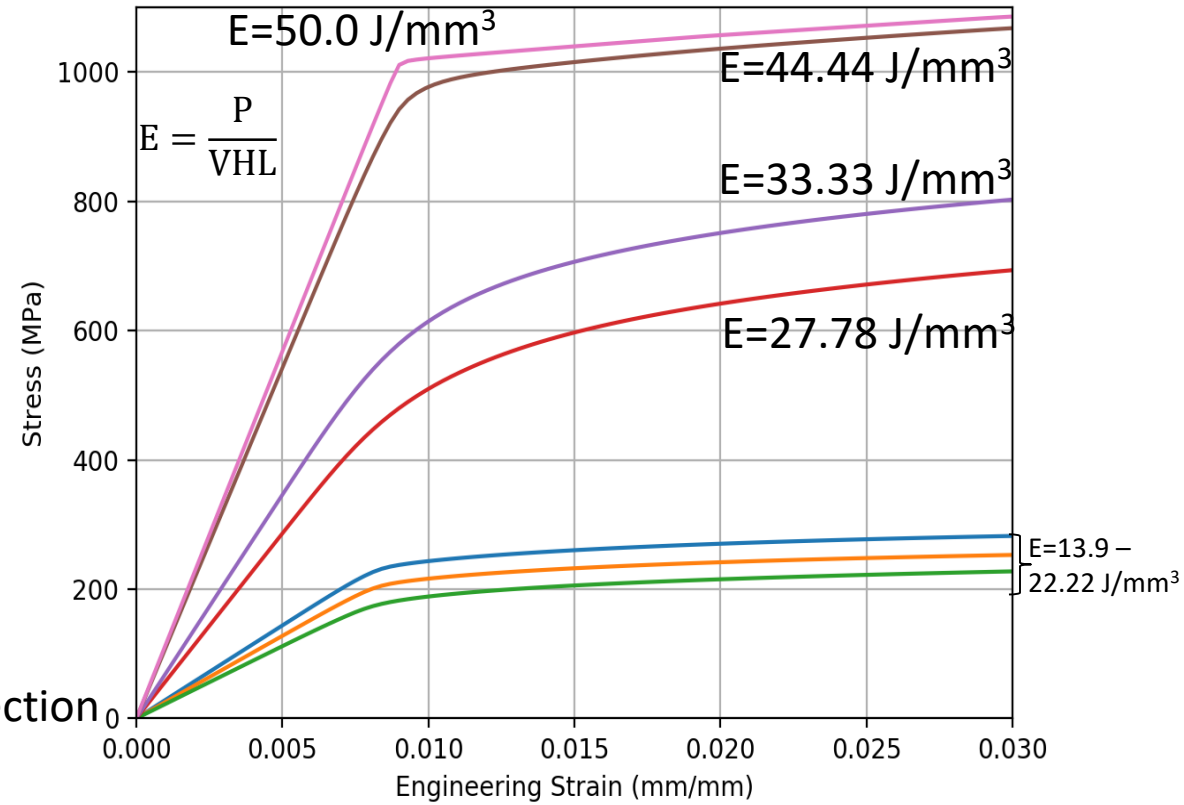
iii) Repeat (i) and (ii) for various combination of process parameters



DEBIT IN MECHANICAL PROPERTIES

- LOF pores of varying energy density.
  - explicitly modelled
  - not homogenized
- No microstructure
- Elastic-plastic, fully dense solid
  - Linear Elastic Isotropic
  - J2 plasticity
- Simple tension out to 3% strain
- Load applied parallel to build direction

Influence of laser energy density (E) on the stress-strain behavior



Material: Ti-6Al-4V

SUMMARY AND CONCLUSIONS

National Institute of Aerospace

SUMMARY:

- Strain localizations surrounding idealized keyhole and LoF pores have been studied
- A 3D LoF porosity prediction framework has been developed and partially validated
- A high-fidelity Process-Structure-Property (PSP) framework has been developed for SLM process

CONCLUSIONS:

- An LoF pore accumulates more strain in comparison to a keyhole pore that occupies the same volume
- It has been demonstrated that an increase in LoF porosity decreases performance. This is also in agreement with experiments.

ACKNOWLEDGEMENTS

- This work was supported through the NASA ARMD's TTT project and the IRAD FY2019 project
- Dr. Christapher Lang for insightful discussions on Process-Structure-Property relations in additive materials
- Dr. Albert Cerrone of University of Notre Dame for collaborating in the development of the 3D LoF porosity model

If I had funding, the big problem I would like to pursue is …

- Use machine learning techniques to develop reduced-order PSP models that run at a significantly lower cost and still retain good amount of fidelity in material response.

- Obtain *in-situ* microstructure-based crack growth data to validate microstructure-based fatigue life prediction models