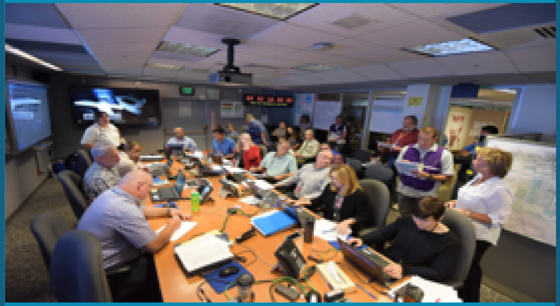
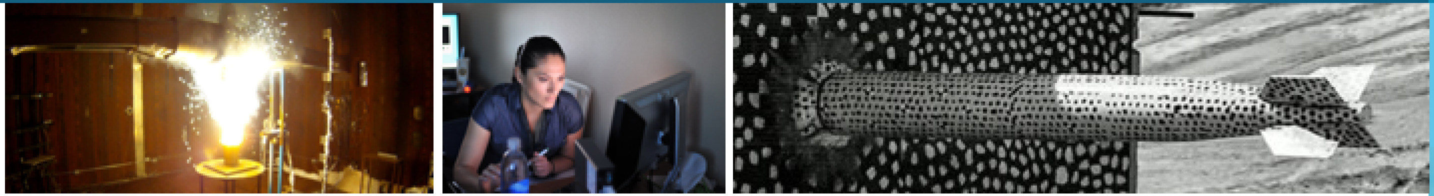
SAND2023-01490C

Data-driven plastic anisotropy predictions using crystal plasticity and deep learning models

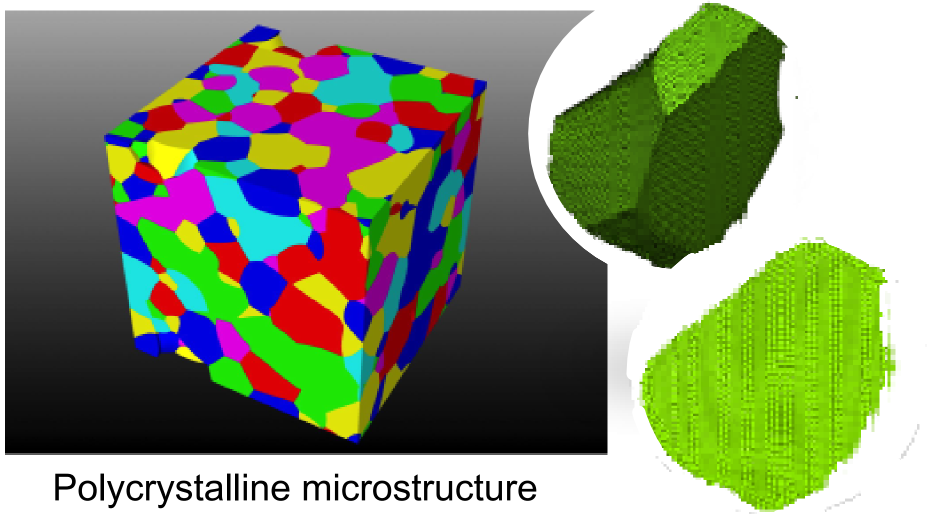




David Montes de Oca Zapiain[1], Hojun Lim[1], Taejoon Park[2], Farhang Pourboghrat[2]

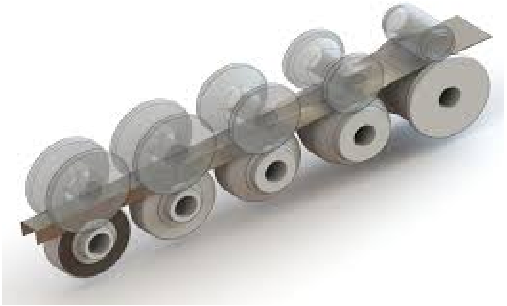
[1]Sandia National Laboratories
[2]The Ohio State University

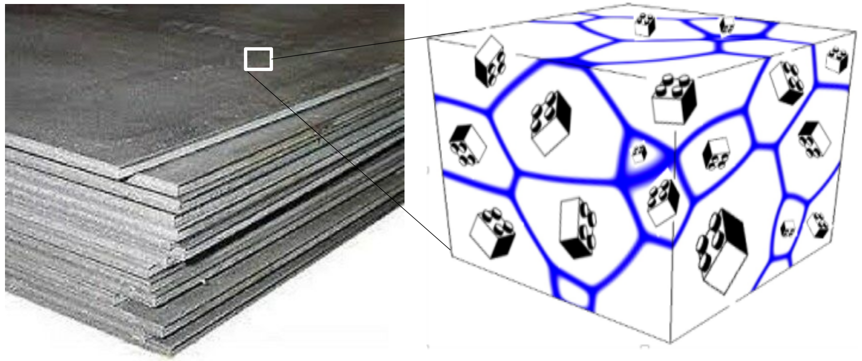
Structure-Property Linkage: Plastic Anisotropy in Metals



Polycrystalline microstructure

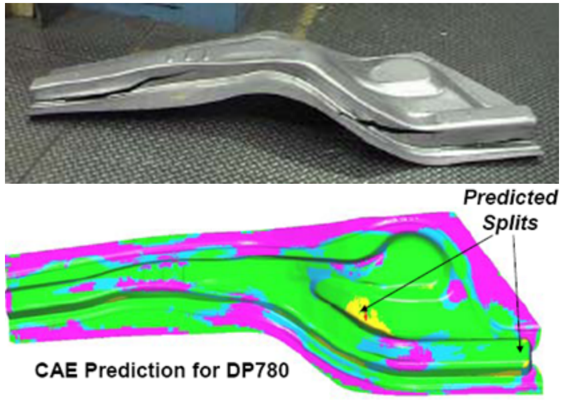
Materials Processing



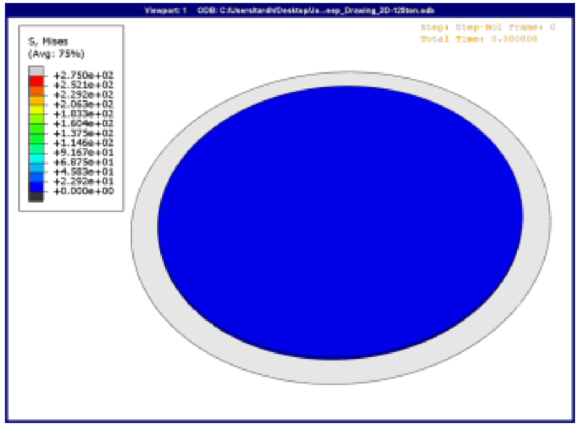


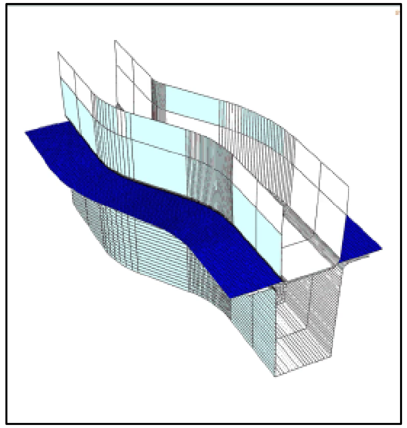
Change in grain morphology and **crystallographic texture**

Accurate strength/formability predictions in metal forming



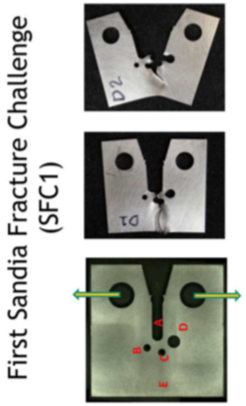
AHSS Workshop, (Stoughton, 2006)

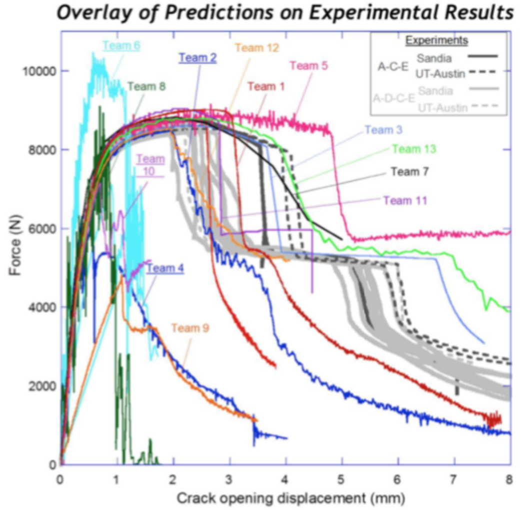




Deep drawing/ Forming simulations

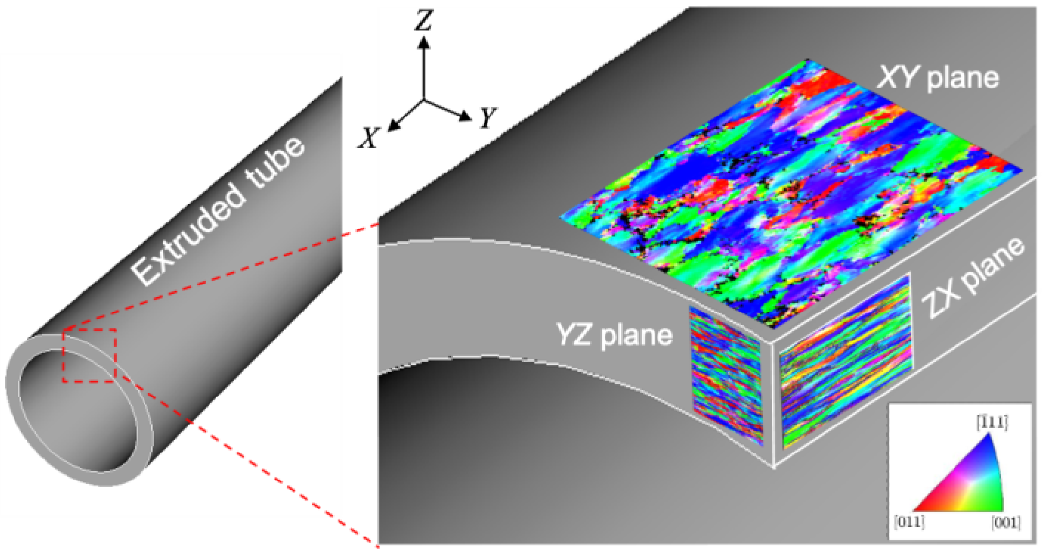
Accurate failure and fracture predictions

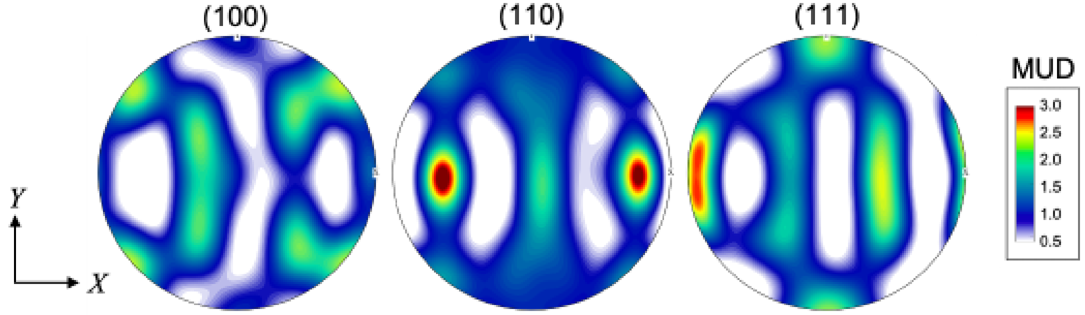




Sandia Fracture Challenge (Kramer et al., 2018)

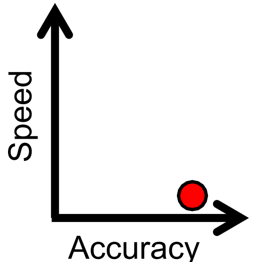
Structure-Property Linkage: Experimental Characterization of Anisotropy – Al7079

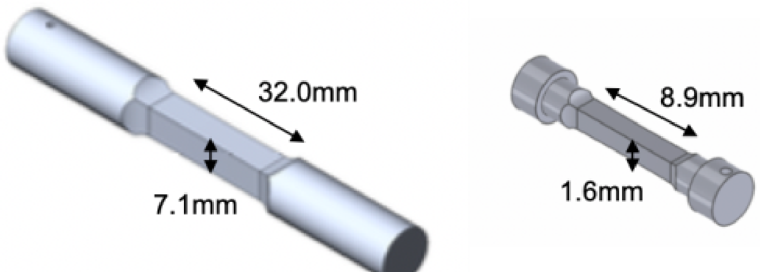




Initial texture

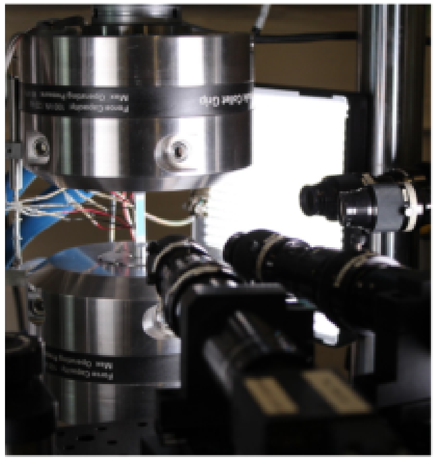
(100), (110) and (111) pole figures from XRD

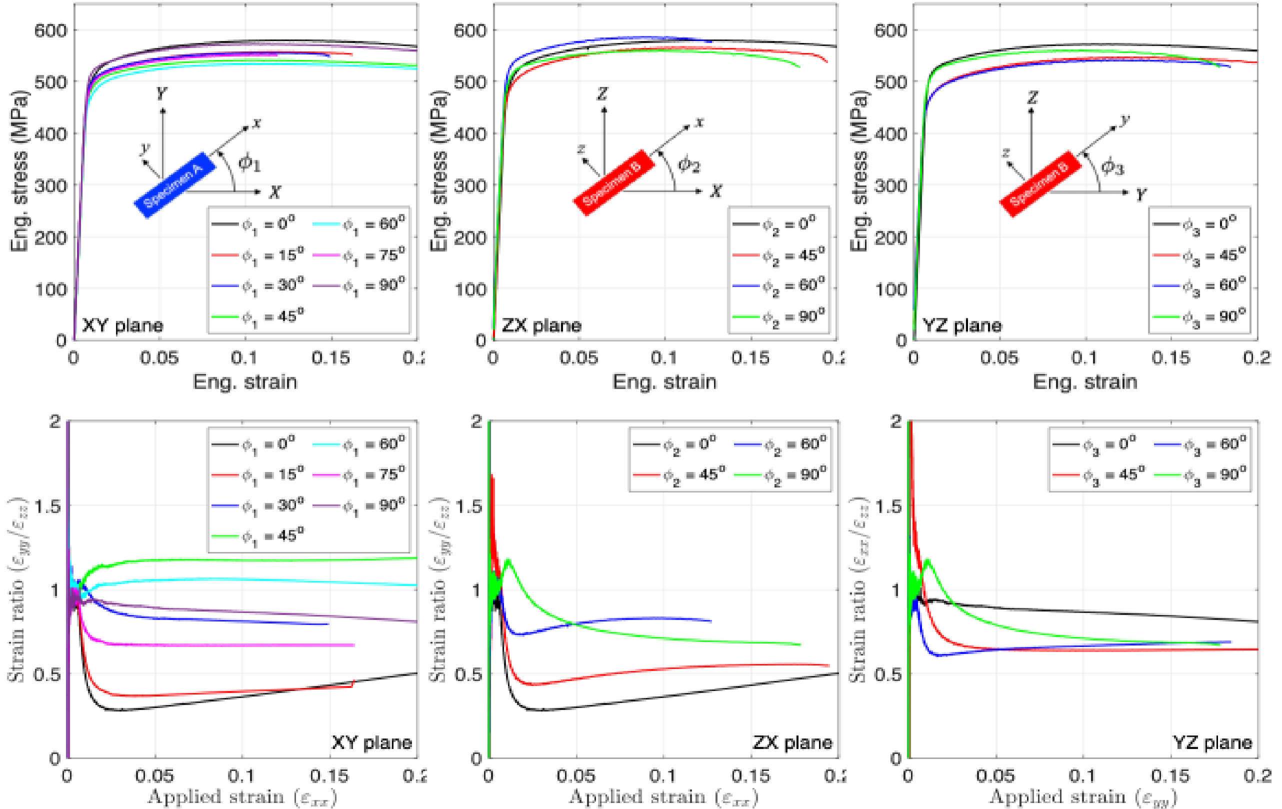




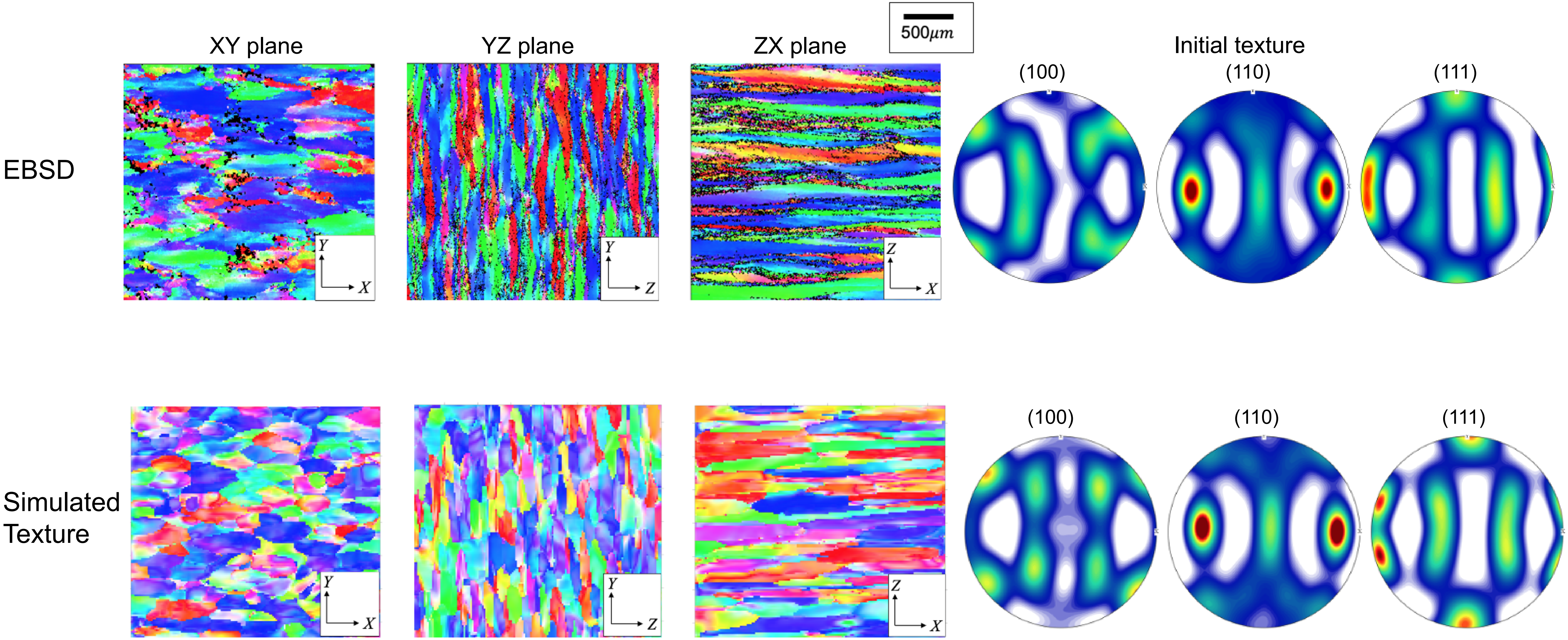
Tensile specimen A (XY plane)

Tensile specimen B (YZ & ZX planes)



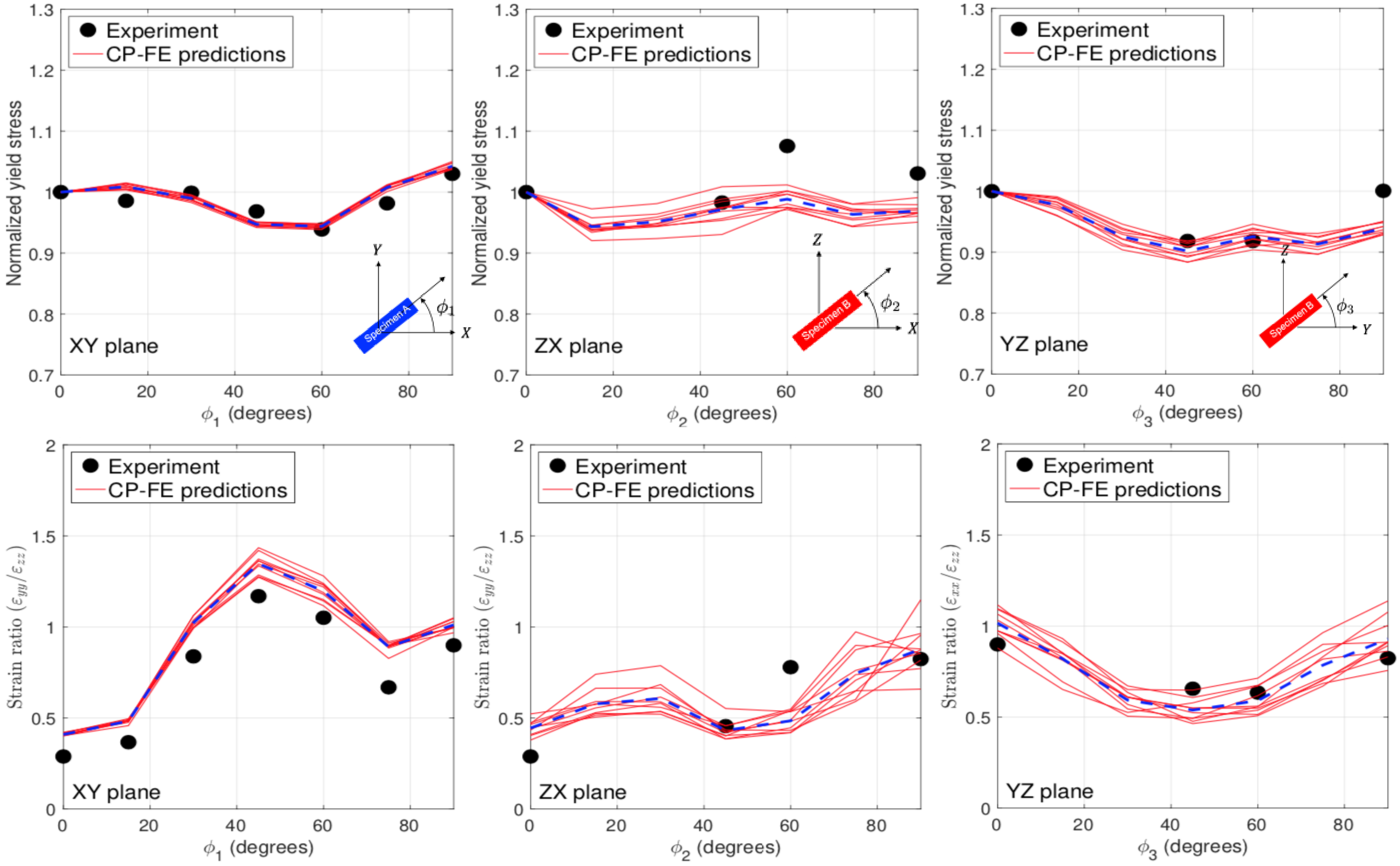


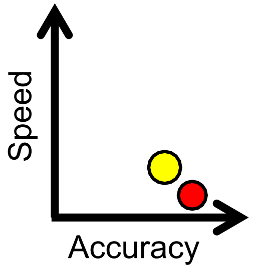
Structure-Property Linkage: *A computational Approach to Anisotropy Characterization*



*Performed extrusion simulations that reproduces measured texture & heterogeneous intragranular features

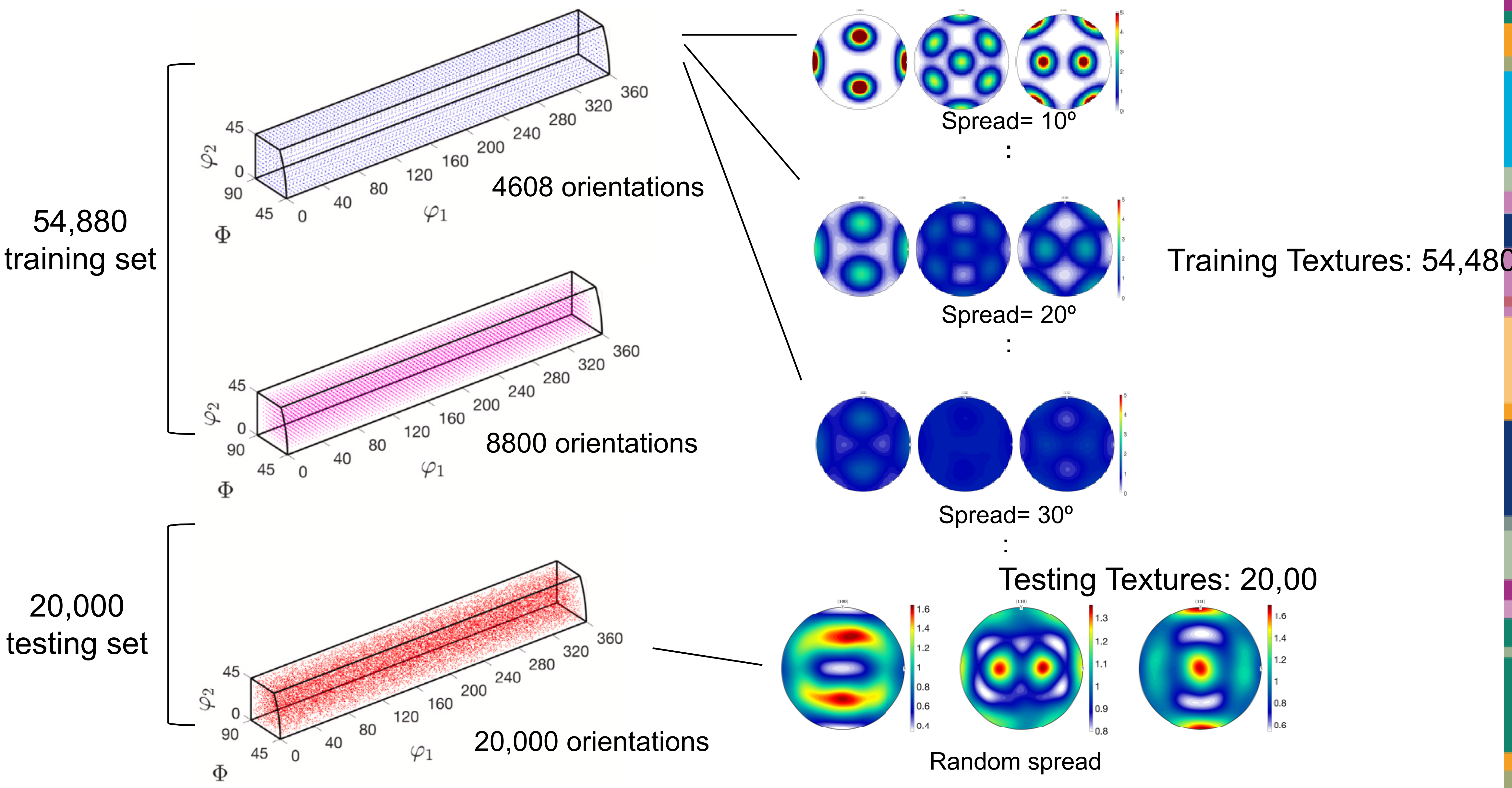
Structure-Property Linkage: *Computational predictions of Yield stress/ lateral strain ratio*





Park et al., MSMSE 2021

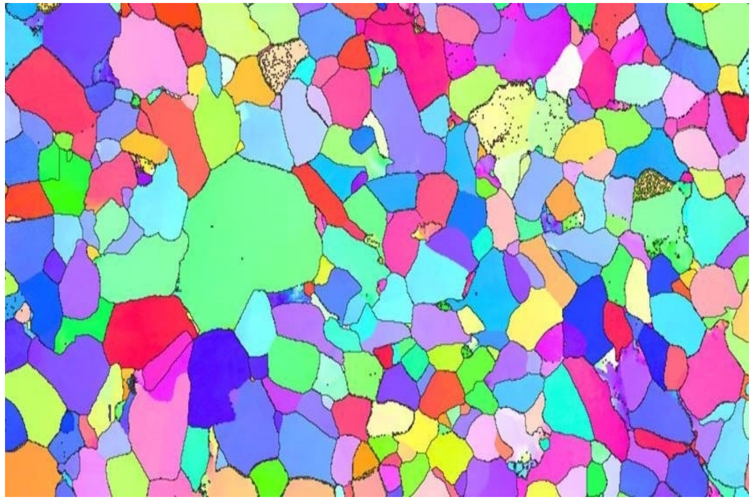
Structure-Property Linkage: *Using computational approaches to generate diverse training sets*

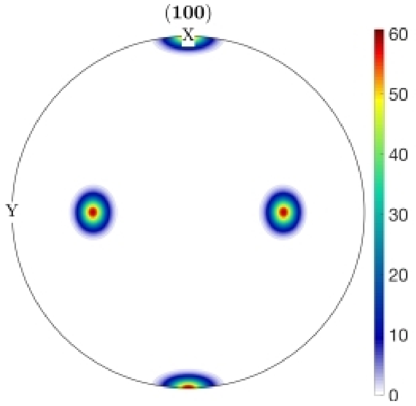


Montes de Oca Zapiain et al., MSE A (2022)

Surrogate Model: *Obtaining Fingerprint Descriptor*

Colors denote the crystal lattice orientation





$f_s(g)$ is the probability distribution of the orientation of the crystal lattice.

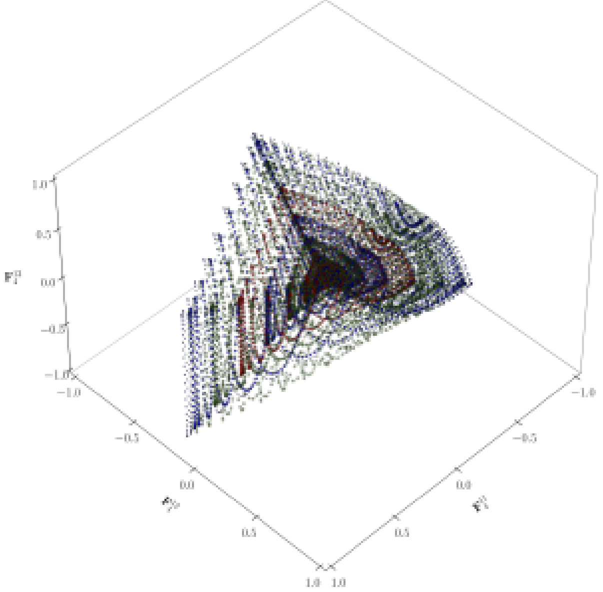
Fourier Series Representation:

$$T_l^{mn}(g) = T_l^{mn}(\varphi_1, \Phi, \varphi_2) = e^{im\varphi_1} P_l^{mn}(\Phi) e^{in\varphi_2}$$

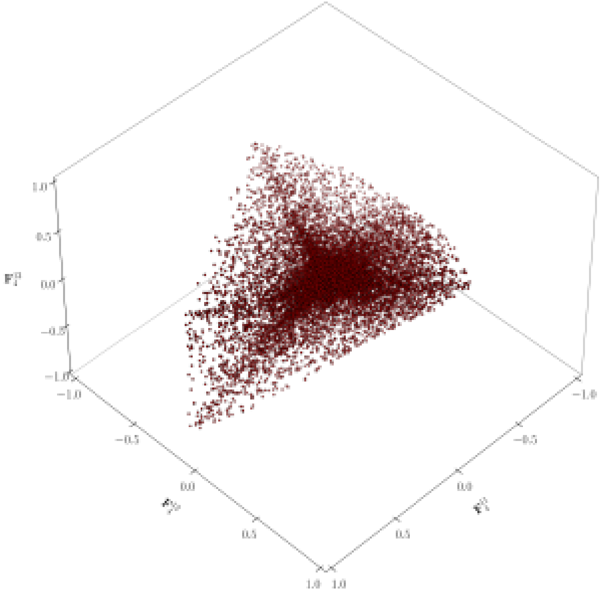
$$f_s(g) = \sum_{\mu,n,l} F_{ls}^{\mu n} T_l^{\mu n}(g),$$

$$F_{ls}^{\mu n} = (2l+1)\int_{FZ} f_s(g) T_l^{\mu n*}(g) dg$$

- Orthogonal Basis functions basis functions
- Customized to account for symmetry.

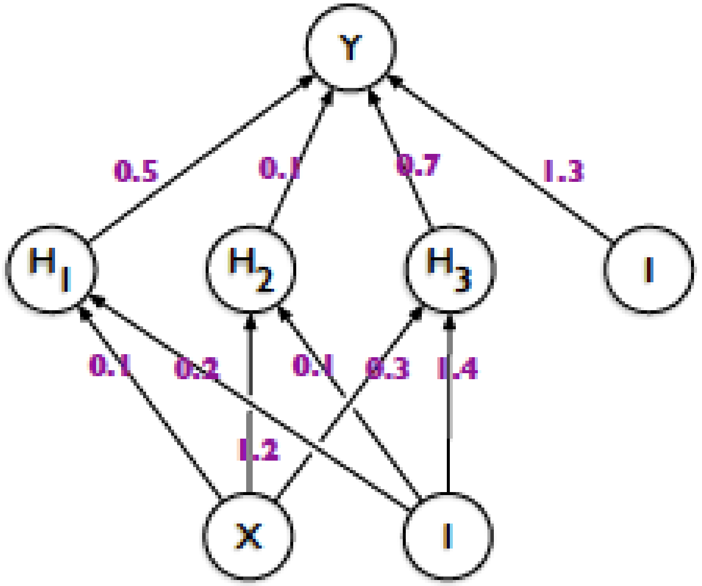


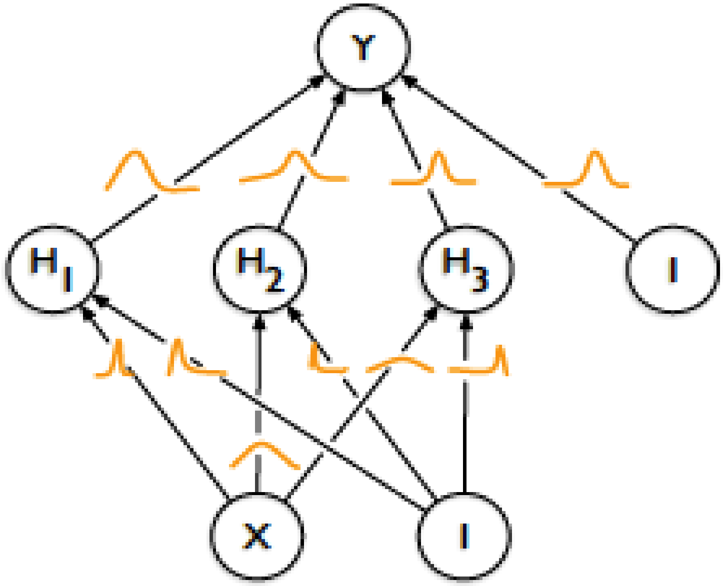
GSH representation of Training Textures



GSH representation of Testing Textures

Surrogate Model: *Neural Network Linkage*



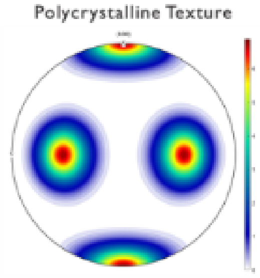


- Architecture of 2 hidden layers with 81 nodes on each layer and sigmoid activation function to predict the output with a GSH truncation level of l=12.
- Monte Carlo Sampling of 50 samples to obtain the distribution of weights, which in turn yielded a distribution of output values.
- Architecture trained to 5000 epochs.

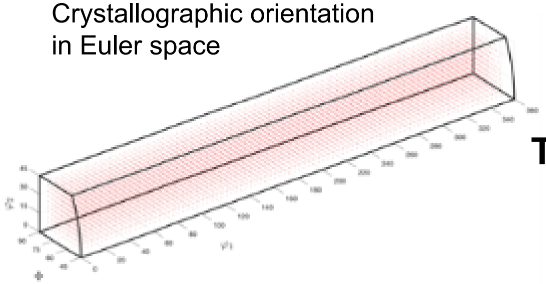
[Blundell et al. (2015)]

Deep Learning Anisotropy Predictions: *Hill's model*

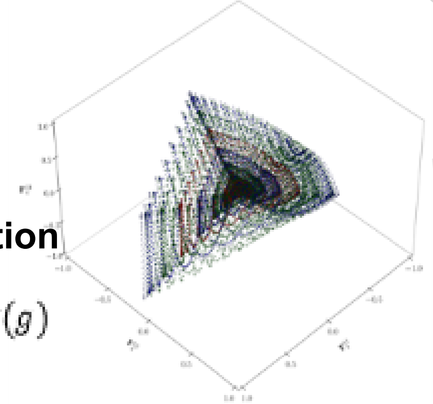
Crystallographic textures



Crystallographic orientation in Euler space



Texture quantification

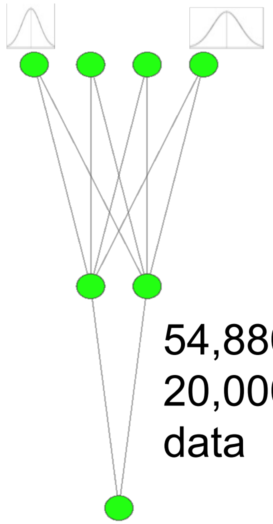


$$f(g) = \sum_{\mu,n,l} F_l^{\mu n} T_l^{\mu n}(g)$$

54,880 textures represented by generalized spherical harmonics (GSH)

$$T_l^{mn}(g) = T_l^{mn}(\varphi_1, \Phi, \varphi_2) = e^{im\varphi_1} P_l^{mn}(\Phi) e^{in\varphi_2}$$

Variation Bayesian Inference Neural Network Model

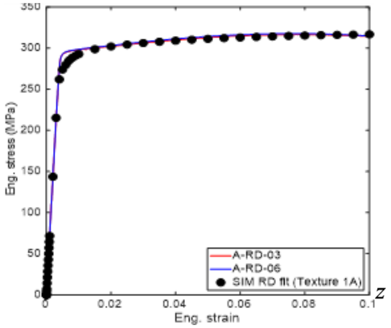


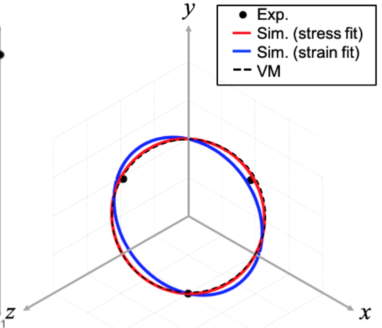
54,880 training data
20,000 validation data

Anisotropy Constants

Crystal plasticity simulations

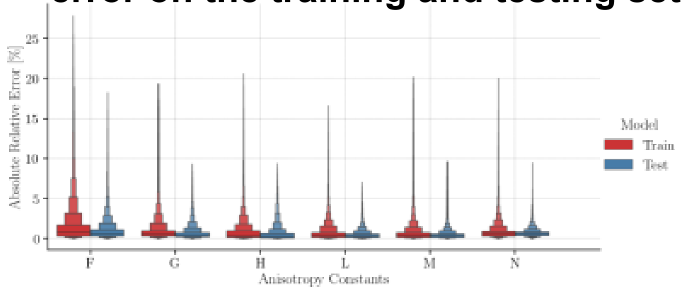
54,880 crystal plasticity simulations performed to investigate anisotropic yield behavior and to fit Hill's anisotropy yield model





$$f = F\left(\sigma_{yy} - \sigma_{zz}\right)^2 + G\left(\sigma_{zz} - \sigma_{xx}\right)^2 + H\left(\sigma_{xx} - \sigma_{yy}\right)^2 + 2\left(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2\right)$$

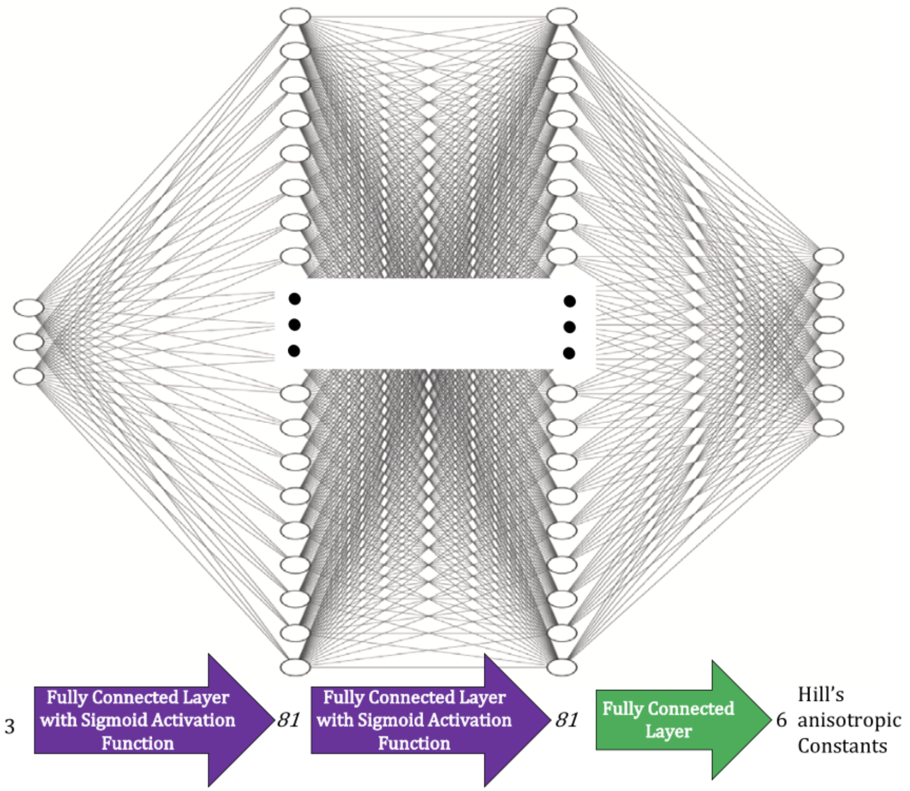
Distribution of absolute relative error on the training and testing set

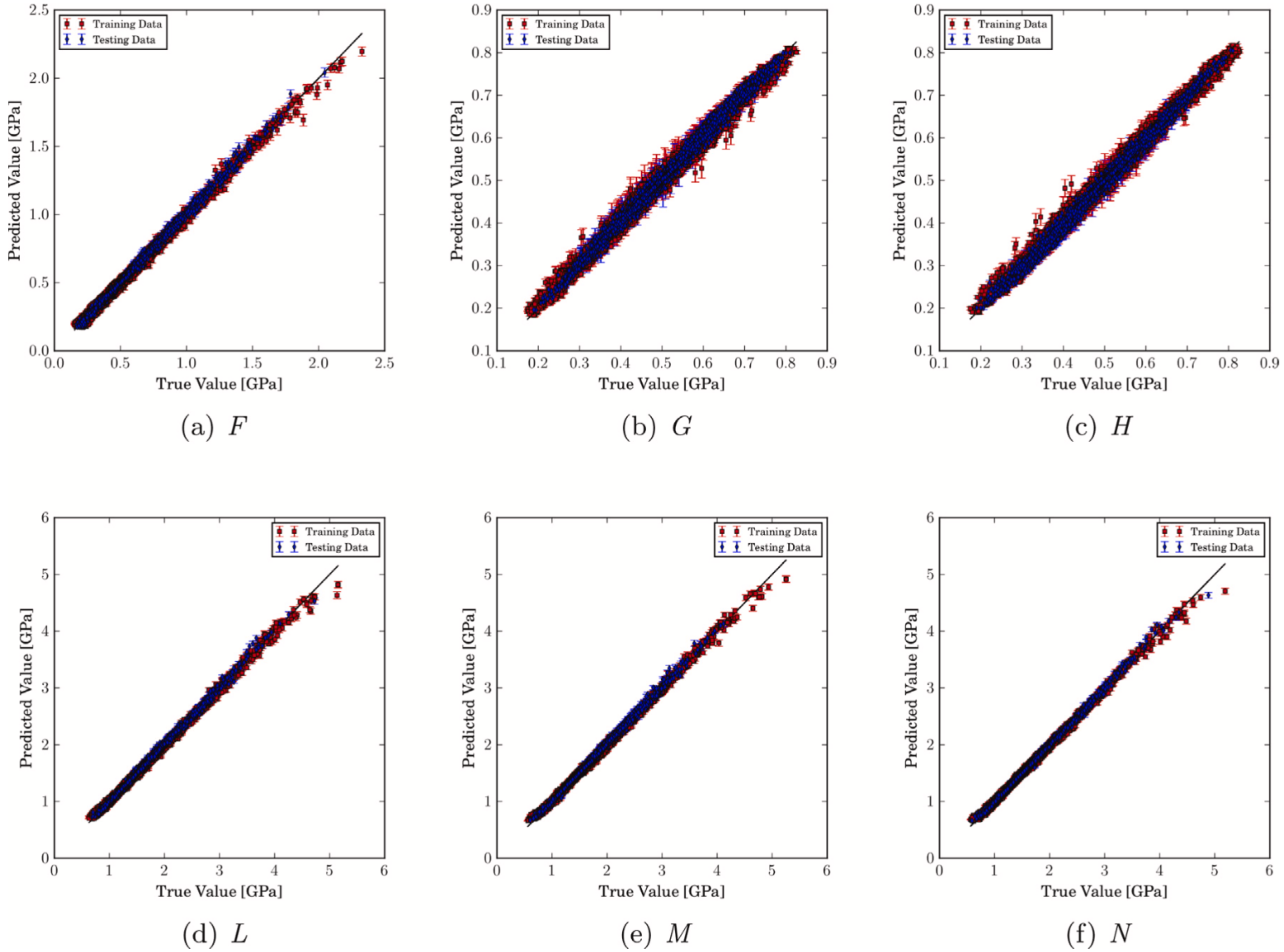


The mean error = 0.63%

Montes de Oca Zapiain et al., MSE-A 2022

Deep Learning Model: *Results*



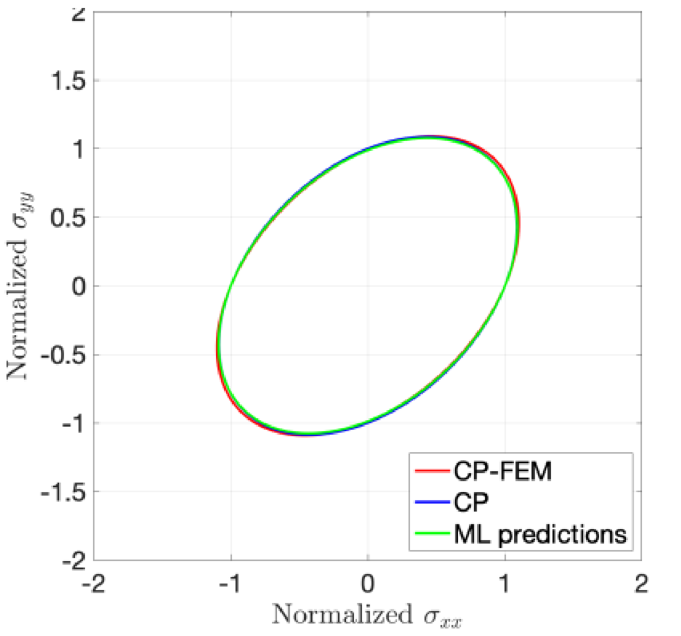


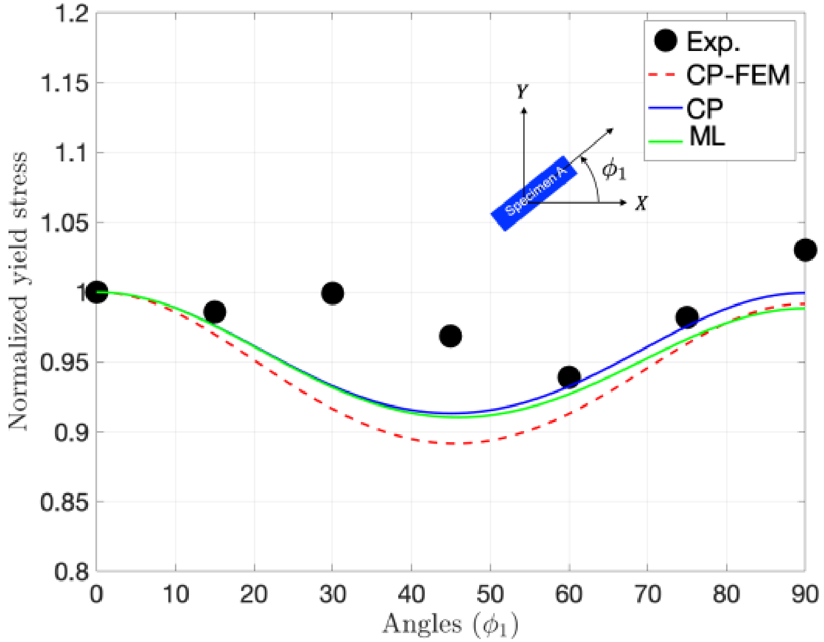
$$f = F\left(\sigma_{yy} - \sigma_{zz}\right)^2 + G\left(\sigma_{zz} - \sigma_{xx}\right)^2 + H\left(\sigma_{xx} - \sigma_{yy}\right)^2 + 2\left(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2\right)$$

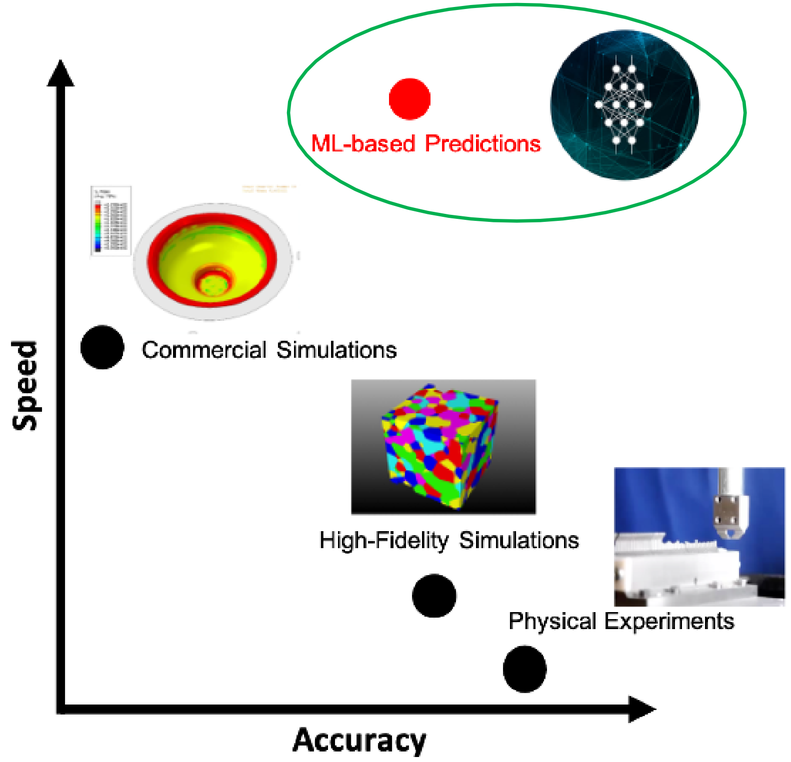
Deep Learning Model: *Comparisons with Experiments & CP simulations*

Parameterizing Hill's quadratic anisotropic yield model: $f = F(\sigma_{yy} - \sigma_{zz})^2 + G(\sigma_{zz} - \sigma_{xx})^2 + H(\sigma_{xx} - \sigma_{yy})^2 + 2(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2)$

Al7079	*F*	*G*	*H*	*L*	*M*	*N*
Crystal plasticity-FE (10 avg.)	0.5961	0.5788	0.4212	1.6133	1.8279	1.9291
Crystal plasticity (no FE)	0.6078	0.6067	0.3933	1.8898	1.7352	1.7920
Neural Network predictions	0.6225 ±0.0018	0.5984 ±0.0013	0.4016 ±0.0013	1.9128 ±0.0017	1.8355 ±0.0018	1.8035 ±0.0022







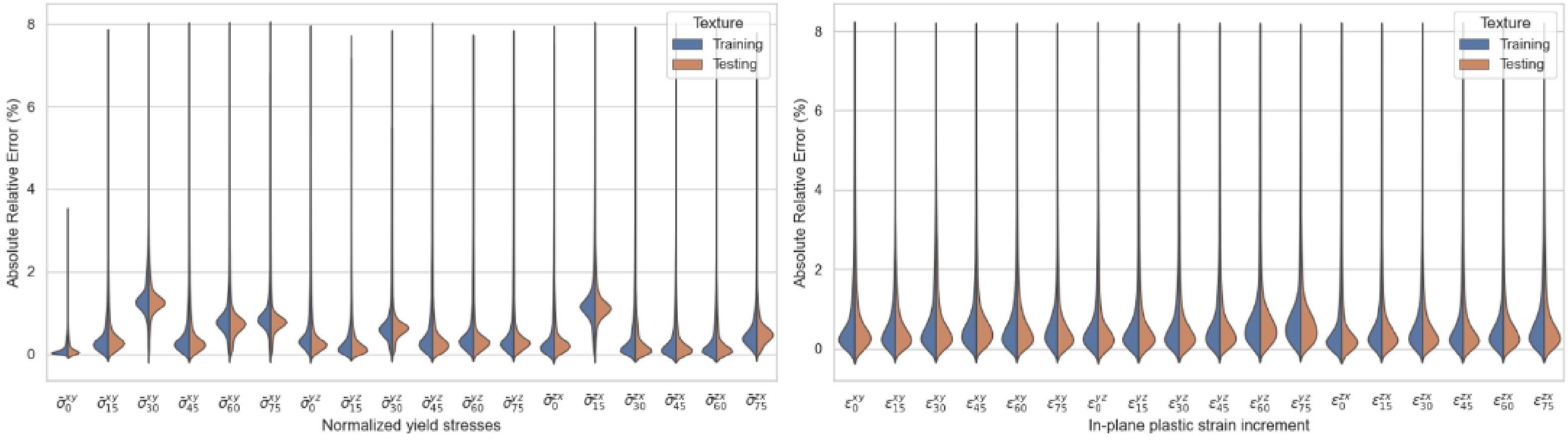
Variation Bayesian Inference Neural Network (VBI-NN) model of Hill's anisotropy model saves computational cost by an order of 1000 compared to crystal plasticity finite element simulations.

Deep Learning Model: *Generalized Anisotropy*

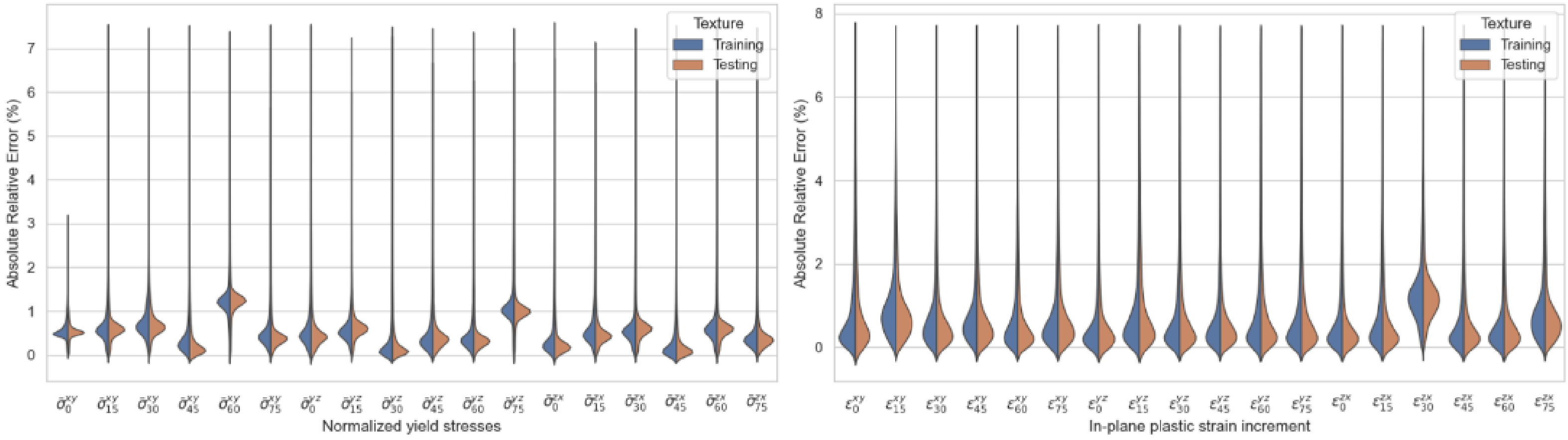
54,880 textures ➡ 54 anisotropy parameters: 18 normalized yield stresses and 36 lateral strain increments

CP vs. ML error:

$$(Error_i)_j = \frac{\left|\left(y_i^{NN}\right)_j - \left(y_i^{CP}\right)_j\right|}{\sum_{j=1}^{N_{texture}} \left(y_i^{CP}\right)_j} \times 100\%$$



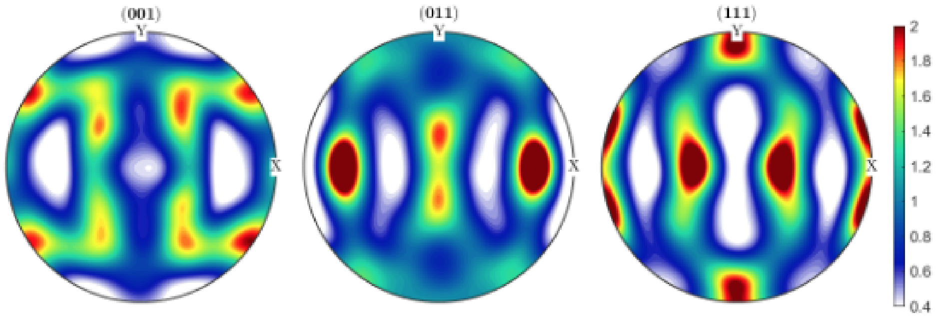
(a) FCC



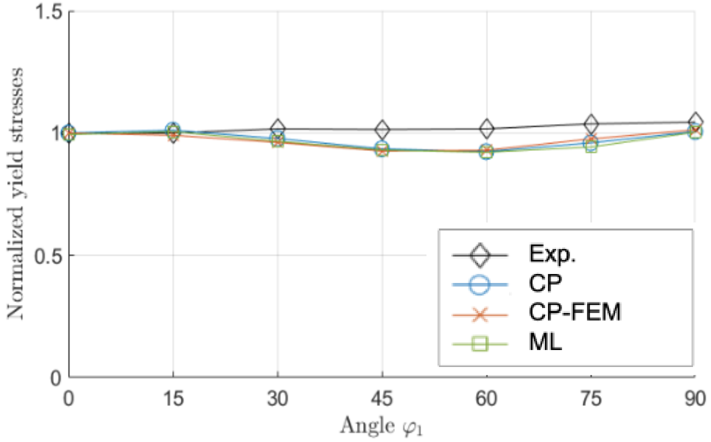
(b) BCC

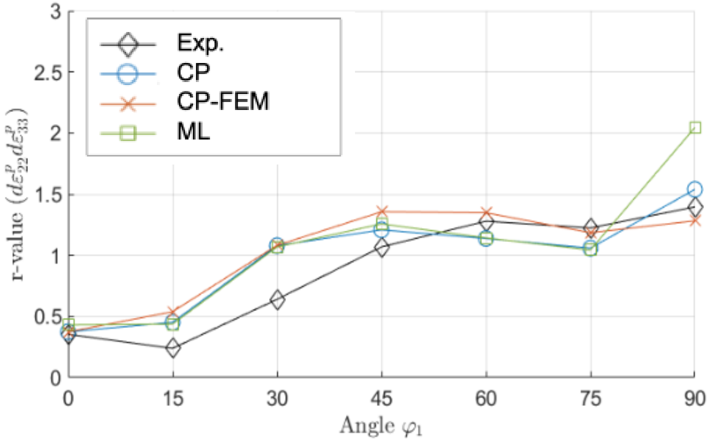
Deep Learning Model: *Application to Al5053 and Al7079*

AA5053

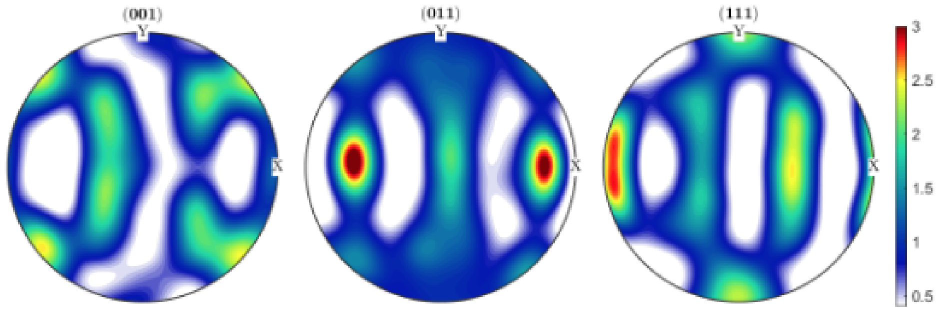


Initial texture

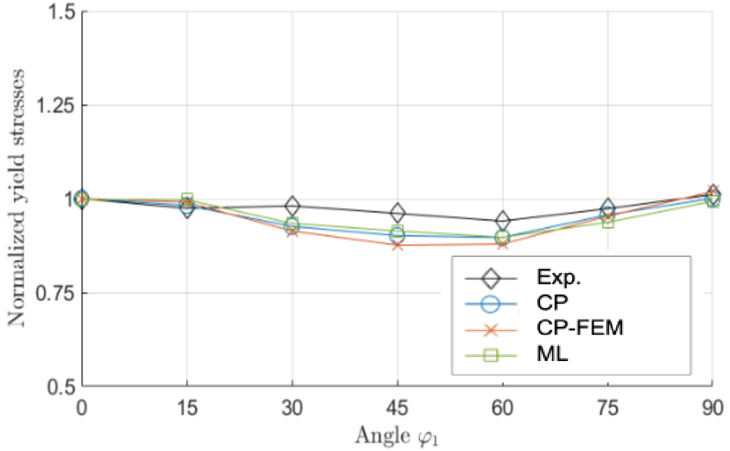


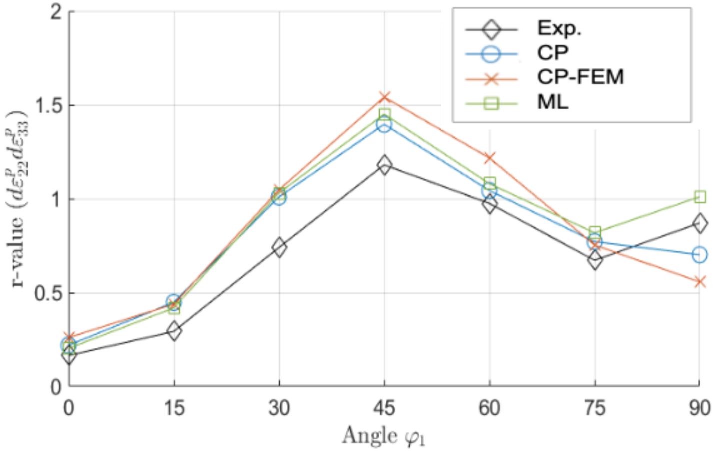


AA7079



Initial texture



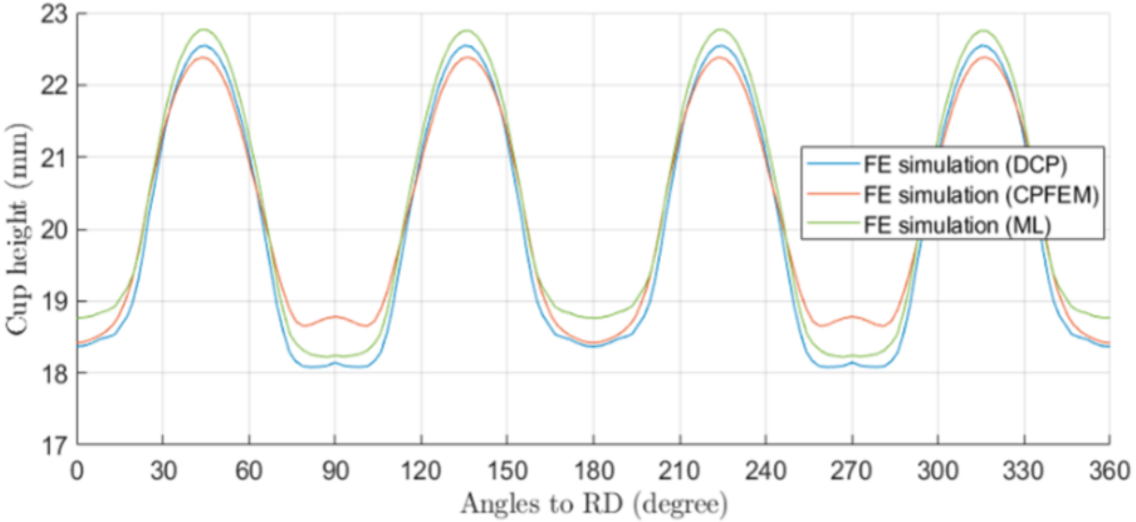


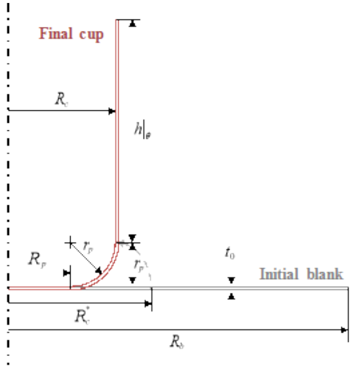
Deep Learning Model: *Application to Cup Drawing FE Simulation*

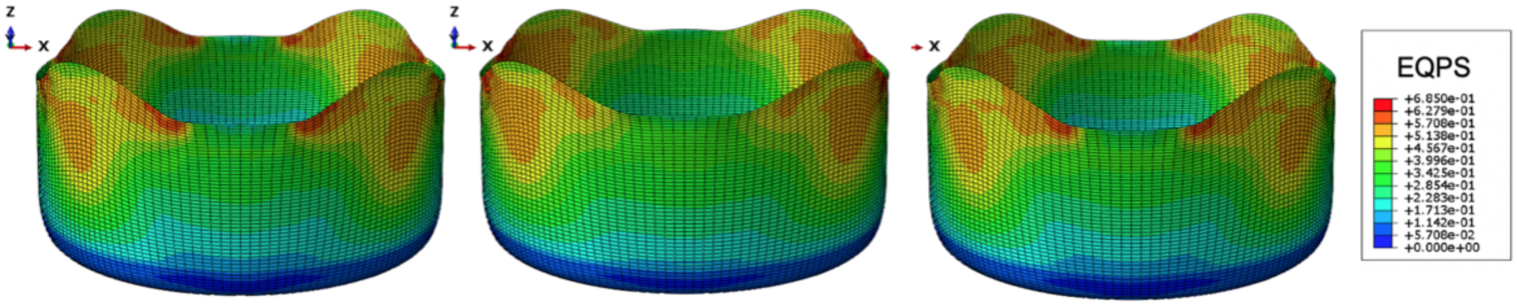
Yld2004-18p parameters for AA5053 & AA7079

Material	AA5042			AA7079		
Input data	ACP	CPFEM	DL	ACP	CPFEM	DL
m	8	8	8	8	8	8
C'_{12}	0.4619	0.2464	0.6263	1.0509	0.4302	0.7625
C'_{13}	0.8858	1.1305	0.9573	0.5351	1.1655	0.1462
C'_{21}	0.9848	1.0584	0.9338	1.1182	1.1990	0.7825
C'_{23}	1.2299	1.1221	1.2882	1.3488	1.2892	1.2530
C'_{31}	0.3762	0.3040	0.4930	1.0426	0.3258	1.1727
C'_{32}	1.3049	1.3922	1.1947	0.6300	1.2479	0.4980
C'_{44}	0.7878	0.4345	0.9902	1.2469	0.5231	1.0684
C'_{55}	1.6519	1.7722	1.1685	1.1925	1.7180	1.1753
C'_{66}	0.7217	0.8402	0.7628	1.4531	0.9517	0.8235
C''_{12}	0.7663	0.6731	0.8781	0.7356	0.5512	0.5213
C''_{13}	1.1852	1.2779	0.9823	1.2552	1.1326	1.0376
C''_{21}	0.8840	0.5907	0.9893	0.5836	0.8244	0.1518
C''_{23}	0.3346	0.1738	0.4572	1.2941	0.5072	-0.7896
C''_{31}	1.3246	1.1097	1.2353	0.7653	1.1498	0.4781
C''_{32}	0.6090	0.2081	0.7023	0.5736	0.4899	-0.7788
C''_{44}	1.2503	1.5792	1.0723	0.8948	1.4978	1.1589
C''_{55}	0.3369	0.0008	0.8386	0.8995	0.2875	1.0046
C''_{66}	1.3630	1.2791	1.3378	0.6968	1.2489	1.4670

Earing profiles of Al5053







Analytical CP
CPFEM
NN

ABAQUS/Explicit
4-node shell element
Blank holding force = 8.9 kN

Energy I-CORPS: *Developing Data-Driven Frameworks Collaboratively*

ENERGY I-CORPS
U.S. Department Of Energy

NNSA
National Nuclear Security Administration

Energy I-CORPS: *Knowledge Sharing with Industry and Academia*

75 Interviews
125 Interviewees
43 Institutions
8 Countries

Industry Lag Time
Up to 6 months and specialized equipment to test materials.

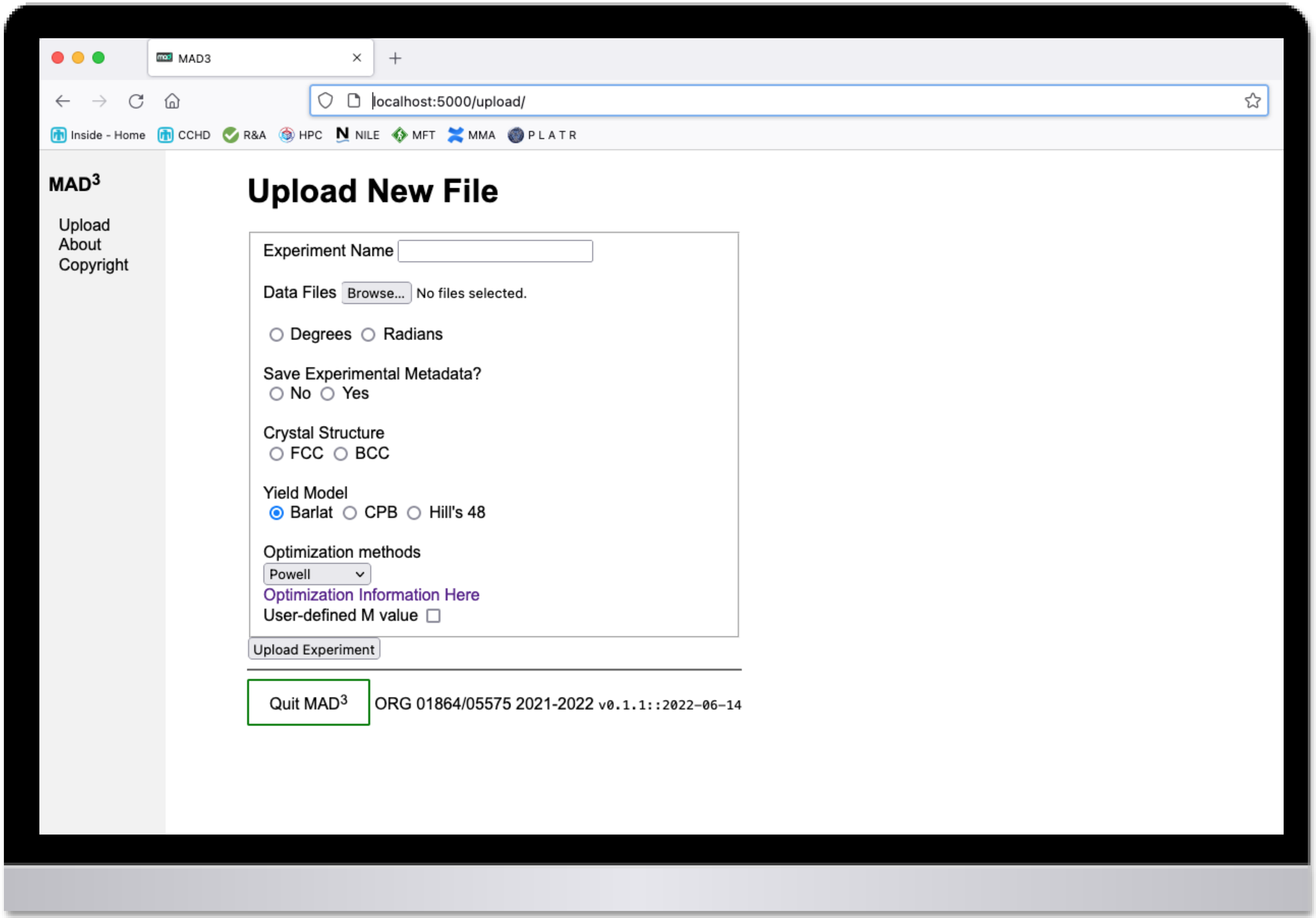
Forced to Use Existing Data
Use anisotropy measurements from a database of previously performed characterizations.

Capital intensive solution
Resultant simulations are not accurate. Consequently, need to perform forming trials.
As a result, current efforts to predict a material's anisotropy from initial microstructure can cost \$2M-\$5M/year per plant.

Massive Carbon Footprint
Mechanical test requires wasting tons of materials, transporting materials, and disposing of wasted materials.

MAD^3: *Packaging our research work into a easy-to-use GUI*

Mac/Windows compatible



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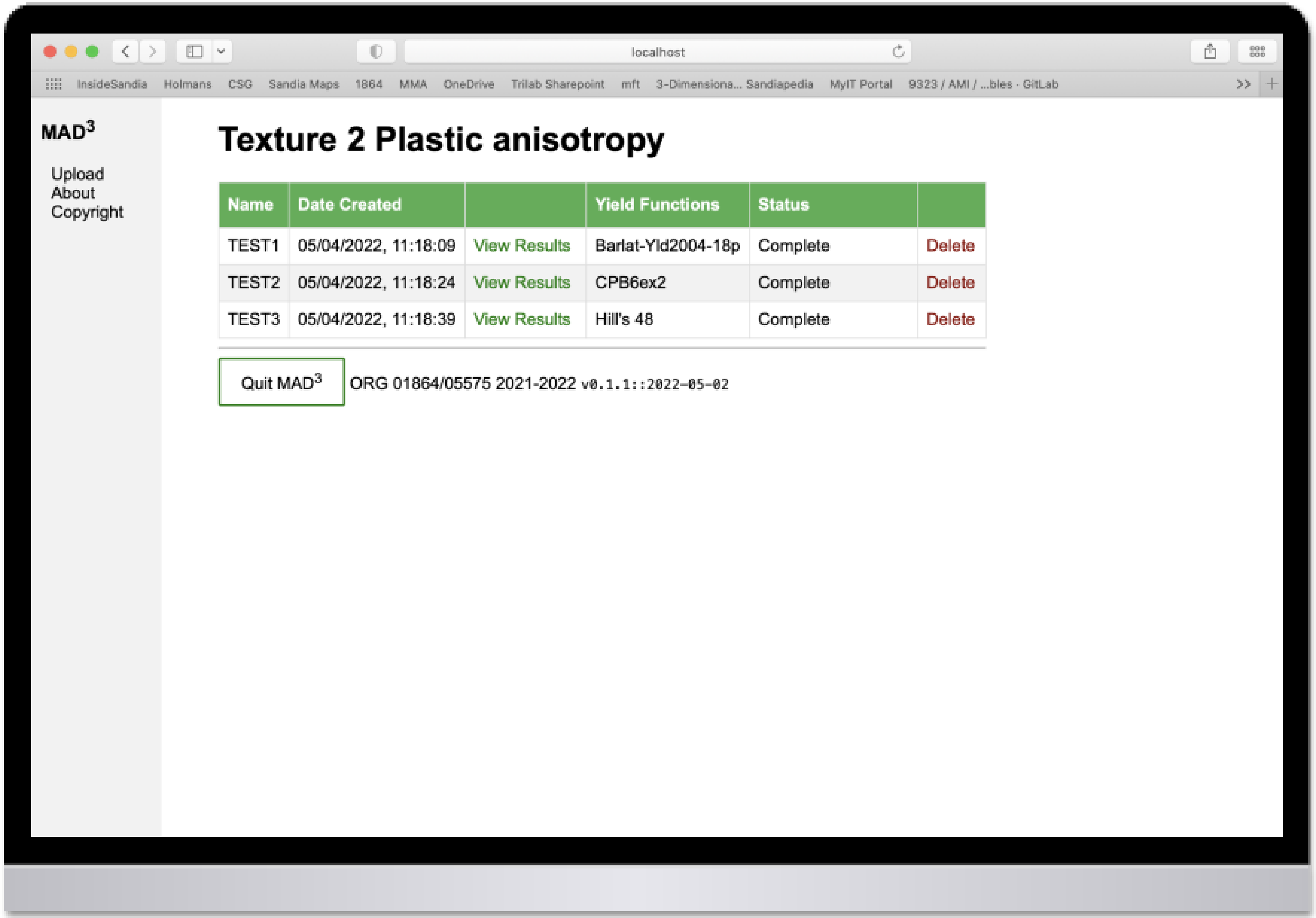
MAD^3: *Packaging our research work into a easy-to-use GUI*

material data driven design

Mac/Windows compatible



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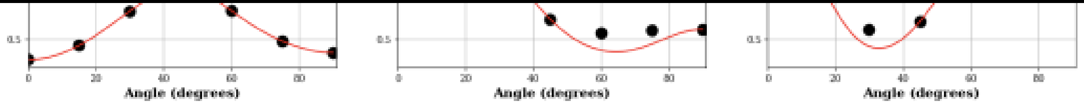
MAD^3: *Packaging our research work into a easy-to-use GUI*

material data driven design

Mac/Windows compatible



Normalized Yield Stress

σ^{xy}_{00}	σ^{xy}_{15}	σ^{xy}_{30}	σ^{xy}_{45}	σ^{xy}_{60}	σ^{xy}_{75}	σ^{yz}_{00}	σ^{yz}_{15}	σ^{yz}_{30}	σ^{yz}_{45}	σ^{yz}_{60}	σ^{yz}_{75}	σ^{zx}_{00}	σ^{zx}_{15}	σ^{zx}_{30}	σ^{zx}_{45}	σ^{zx}_{60}	σ^{zx}_{75}
1.0	0.9942	0.9738	0.9745	0.9853	1.0152	1.038	1.0405	1.0592	1.0578	1.0202	0.9942	0.9928	0.9891	1.0151	1.0817	1.081	1.0304

Lateral Strain 1 (in-plane)

ε^{xy}_{00}	ε^{xy}_{15}	ε^{xy}_{30}	ε^{xy}_{45}	ε^{xy}_{60}	ε^{xy}_{75}	ε^{yz}_{00}	ε^{yz}_{15}	ε^{yz}_{30}	ε^{yz}_{45}	ε^{yz}_{60}	ε^{yz}_{75}	ε^{zx}_{00}	ε^{zx}_{15}	ε^{zx}_{30}	ε^{zx}_{45}	ε^{zx}_{60}	ε
-0.2198	-0.3066	-0.4509	-0.5221	-0.4532	-0.3209	-0.7112	-0.6348	-0.5006	-0.3975	-0.3538	-0.3767	-0.6394	-0.5031	-0.3654	-0.3792	-0.552	-0.7

Lateral Strain 2 (normal to plane)

ε^{xy}_{00}	ε^{xy}_{15}	ε^{xy}_{30}	ε^{xy}_{45}	ε^{xy}_{60}	ε^{xy}_{75}	ε^{yz}_{00}	ε^{yz}_{15}	ε^{yz}_{30}	ε^{yz}_{45}	ε^{yz}_{60}	ε^{yz}_{75}	ε^{zx}_{00}	ε^{zx}_{15}	ε^{zx}_{30}	ε^{zx}_{45}	ε^{zx}_{60}	ε
-0.7768	-0.7021	-0.5684	-0.4985	-0.5649	-0.6668	-0.2544	-0.3155	-0.4485	-0.5569	-0.6247	-0.6294	-0.3868	-0.5181	-0.603	-0.5507	-0.3749	-0.2

Optimized parameters for Barlat Yld2004-18p (Barlat et al., 2005)

c'_12	c'_13	c'_21	c'_23	c'_31	c'_32	c'_44	c'_55	c'_66	c''_12	c''_13	c''_21	c''_23	c''_31	c''_32	c''_44	c''_55	c''_66
0.2358	0.8113	0.7176	0.9674	0.9987	0.9872	0.9212	1.1197	0.8716	1.1107	1.2219	1.0687	0.1918	0.5613	1.1125	0.7516	0.5393	1.0855

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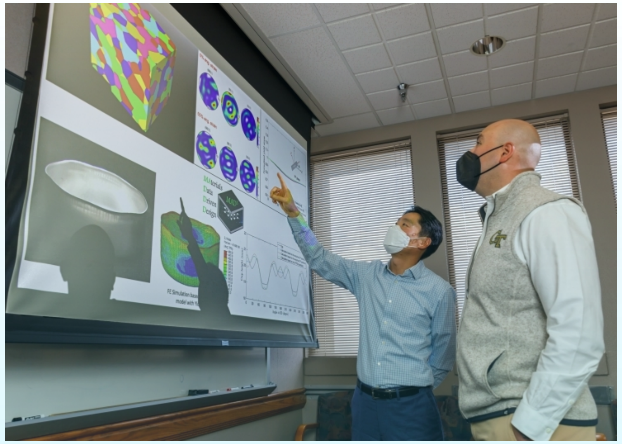
Summary

- CP-FEM simulations provide reasonable yield stresses and lateral strain ratio predictions.

- Deep Learning model was trained from CP data and showed good agreement in anisotropy predictions.

- Developed a GUI-based app that instantly predicts plastic anisotropy from initial texture.

- ML–based model provides a convenient & direct link from *material's* ***microstructure*** to *macro-scale* ***anisotropy*** of metals.



THANK YOU !

https://newsreleases.sandia.gov/quality_testing/

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Yield models

1. Hill 1948 function (6 coefficients) [1]

$$f = \bar{\sigma}^2 = (G+H)\sigma_{xx}^2 + (H+F)\sigma_{yy}^2 + (F+G)\sigma_{zz}^2 - 2\left(F\sigma_{yy}\sigma_{zz} + G\sigma_{zz}\sigma_{xx} + H\sigma_{xx}\sigma_{yy}\right) + 2\left(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2\right)$$

2. Yld2004-18p function (18+1 coefficients) [2]

$$f = 4\bar{\sigma}^a = \left|\tilde{S}'_1 - \tilde{S}''_1\right|^a + \left|\tilde{S}'_1 - \tilde{S}''_2\right|^a + \left|\tilde{S}'_1 - \tilde{S}''_3\right|^a + \left|\tilde{S}'_2 - \tilde{S}''_1\right|^a + \left|\tilde{S}'_2 - \tilde{S}''_2\right|^a + \left|\tilde{S}'_2 - \tilde{S}''_3\right|^a + \left|\tilde{S}'_3 - \tilde{S}''_1\right|^a + \left|\tilde{S}'_3 - \tilde{S}''_2\right|^a + \left|\tilde{S}'_3 - \tilde{S}''_3\right|^a$$

$\tilde{S}'_i$ and $\tilde{S}''_i$ (i=1,2, and 3) are principal components of the linearly transformed deviatoric stresses, $\tilde{\boldsymbol{s}}'$ and $\tilde{\boldsymbol{s}}''$.

$$\tilde{\boldsymbol{s}}' = \begin{bmatrix} s'_{xx} \\ s'_{yy} \\ s'_{zz} \\ s'_{xy} \\ s'_{yz} \\ s'_{zx} \end{bmatrix} = \boldsymbol{C}'\boldsymbol{s} = \begin{bmatrix} 0 & -c'_{12} & -c'_{13} & 0 & 0 & 0 \\ -c'_{21} & 0 & -c'_{23} & 0 & 0 & 0 \\ -c'_{31} & -c'_{32} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c'_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c'_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c'_{66} \end{bmatrix} \begin{bmatrix} s_{xx} \\ s_{yy} \\ s_{zz} \\ s_{yz} \\ s_{zx} \\ s_{xy} \end{bmatrix}$$

3. CPB06ex2 (18+1 coefficients) [3]

$$f = \bar{\sigma}^m = \frac{3^m}{2^{m+1}(1-k)^m + 4(1+k)^m}\left[\left(\tilde{S}'_1 - k\left|\tilde{S}'_1\right|\right)^m + \left(\tilde{S}'_2 - k\left|\tilde{S}'_2\right|\right)^m + \left(\tilde{S}'_3 - k\left|\tilde{S}'_3\right|\right)^m + \left(\tilde{S}''_1 - k\left|\tilde{S}''_1\right|\right)^m + \left(\tilde{S}''_2 - k\left|\tilde{S}''_2\right|\right)^m + \left(\tilde{S}''_3 - k\left|\tilde{S}''_3\right|\right)^m\right]$$

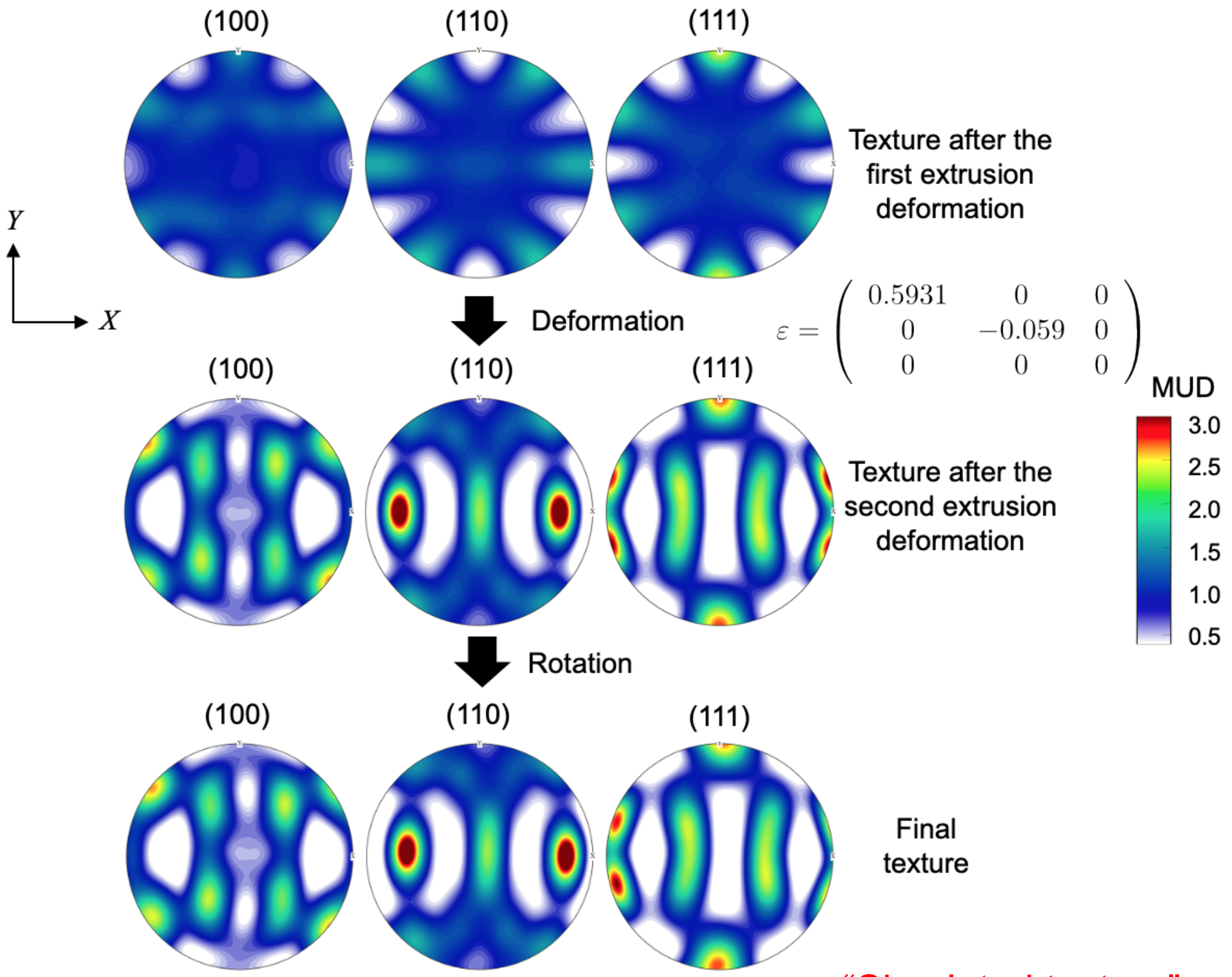
$$\tilde{\boldsymbol{s}}' = \begin{bmatrix} s'_{xx} \\ s'_{yy} \\ s'_{zz} \\ s'_{xy} \\ s'_{yz} \\ s'_{zx} \end{bmatrix} = \boldsymbol{C}'\boldsymbol{s} = \begin{bmatrix} c'_{11} & c'_{12} & c'_{13} & 0 & 0 & 0 \\ c'_{12} & c'_{22} & c'_{23} & 0 & 0 & 0 \\ c'_{12} & c'_{23} & c'_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c'_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c'_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c'_{66} \end{bmatrix} \begin{bmatrix} s_{xx} \\ s_{yy} \\ s_{zz} \\ s_{yz} \\ s_{zx} \\ s_{xy} \end{bmatrix}$$

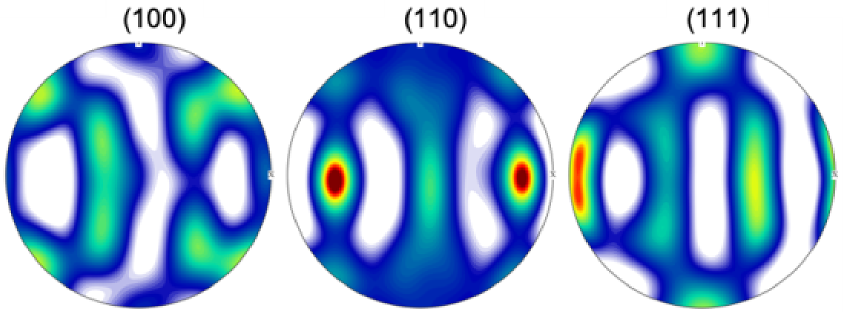
[1] Hill, R., 1948. A Theory of the Yielding and Plastic Flow of Anisotropic Metals, 281-297.
[2] Barlat, F., Aretz, H., Yoon, J.W., Karabin, M.E., Brem, J.C., Dick, R.E., 2005. Linear transformation-based anisotropic yield functions. International Journal of Plasticity 21, 1009-1039.
[3] Plunkett, B., Cazacu, O., Barlat, F., 2008. Orthotropic yield criteria for description of the anisotropy in tension and compression of sheet metals. Int J Plasticity 24, 847-866.

Computational microstructure 2: Simulated texture

CP-FEM typically assumes uniform dislocation distributions and intraganular crystal orientations

Perform extrusion simulations that reproduces measured texture & heterogeneous intragranular features





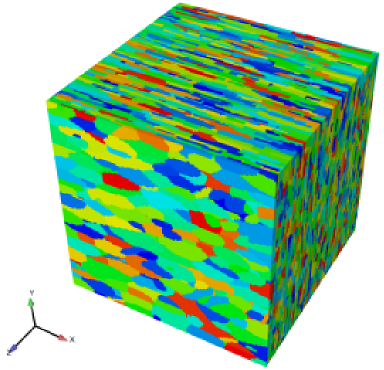
c.f. XRD

"Simulated texture"

Outline

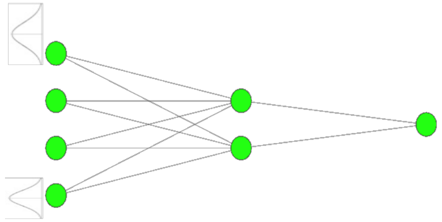
1. Predicting plastic anisotropy using large-scale crystal plasticity finite element simulations[1,2]

   Investigating the effects of heterogeneous microstructural features and constitutive models on plastic anisotropy predictions using crystal plasticity simulations.



2. Predicting plastic anisotropy using Bayesian neural network surrogate models[3,4]

   Developing an efficient data-driven protocol to accurately predict plastic anisotropy from initial crystallographic texture using Variational Bayesian Inference techniques



3. Revolutionizing Manufacturing through Machine Learning

   Revolutionizing the manufacturing process by eliminating the need to perform expensive, timely, and resource heavy mechanical materials test by utilizing the power of machine learning.

[1]Corona et al., IJSS (2021), [2]Park et al., MSMSE (2021), [3]Montes de Oca Zapiain et al., MSE-A (2022), [4]Park et al., (in progress)

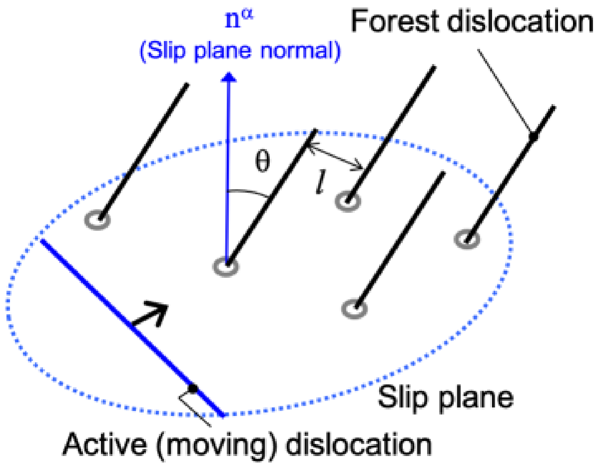
Effects of CP hardening model

Slip resistance: $$g^\alpha = g_0 + A\mu b\sqrt{\sum_{\beta=1}^{12} H^{\alpha\beta}\rho^\beta}$$

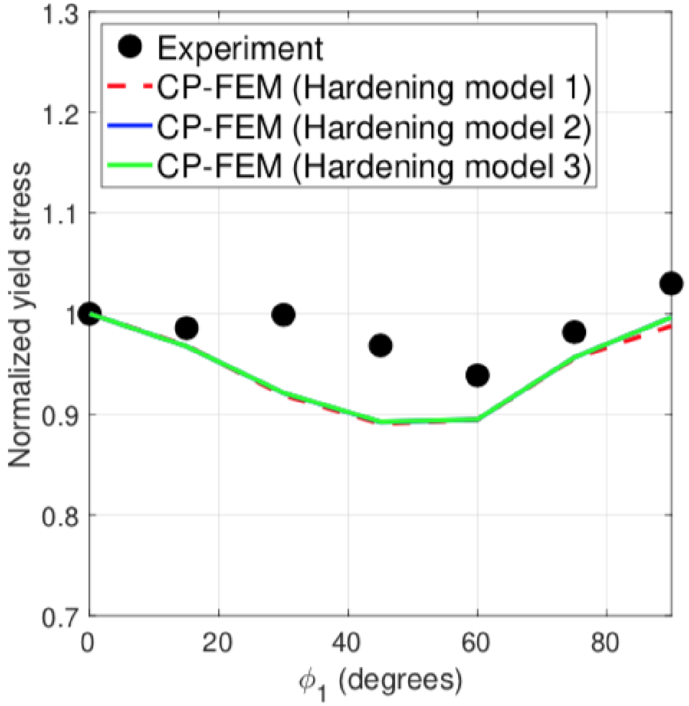
$$H^{\alpha\beta} = 1 \quad \text{(Model 1)}$$

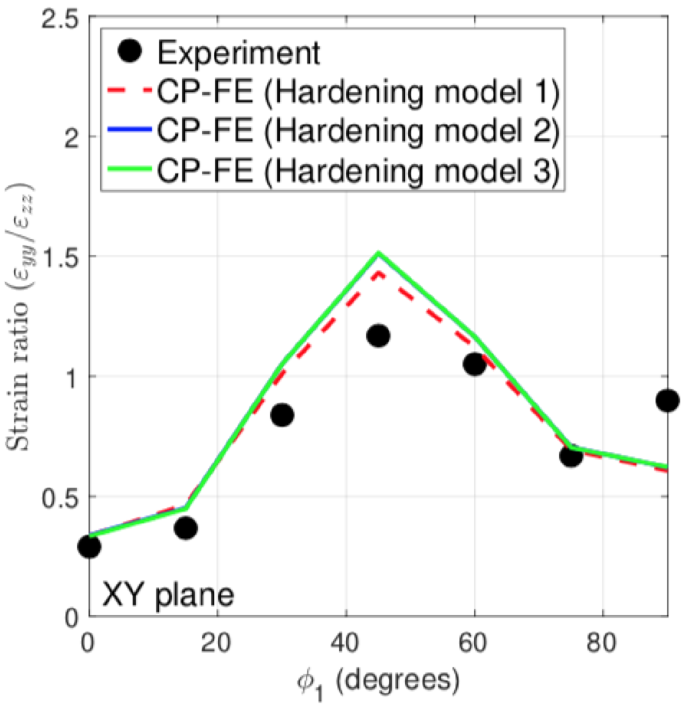
$$H^{\alpha\alpha} = 1 \quad H^{\alpha\beta} = 1.4 \quad \text{(Model 2)}$$

$$H^{\alpha\beta} = \mathbf{n}^\alpha \cdot \xi^\beta \quad \text{(Model 3)}$$

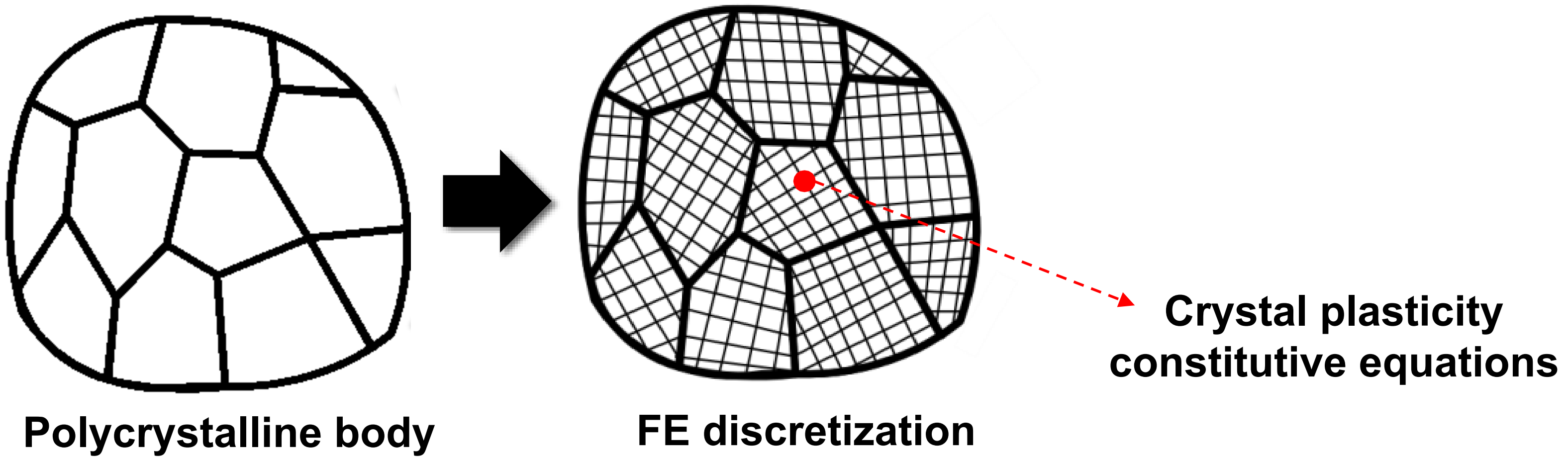


Lee et al., IJP (2010)





Crystal Plasticity – Finite Element (CP-FE) method



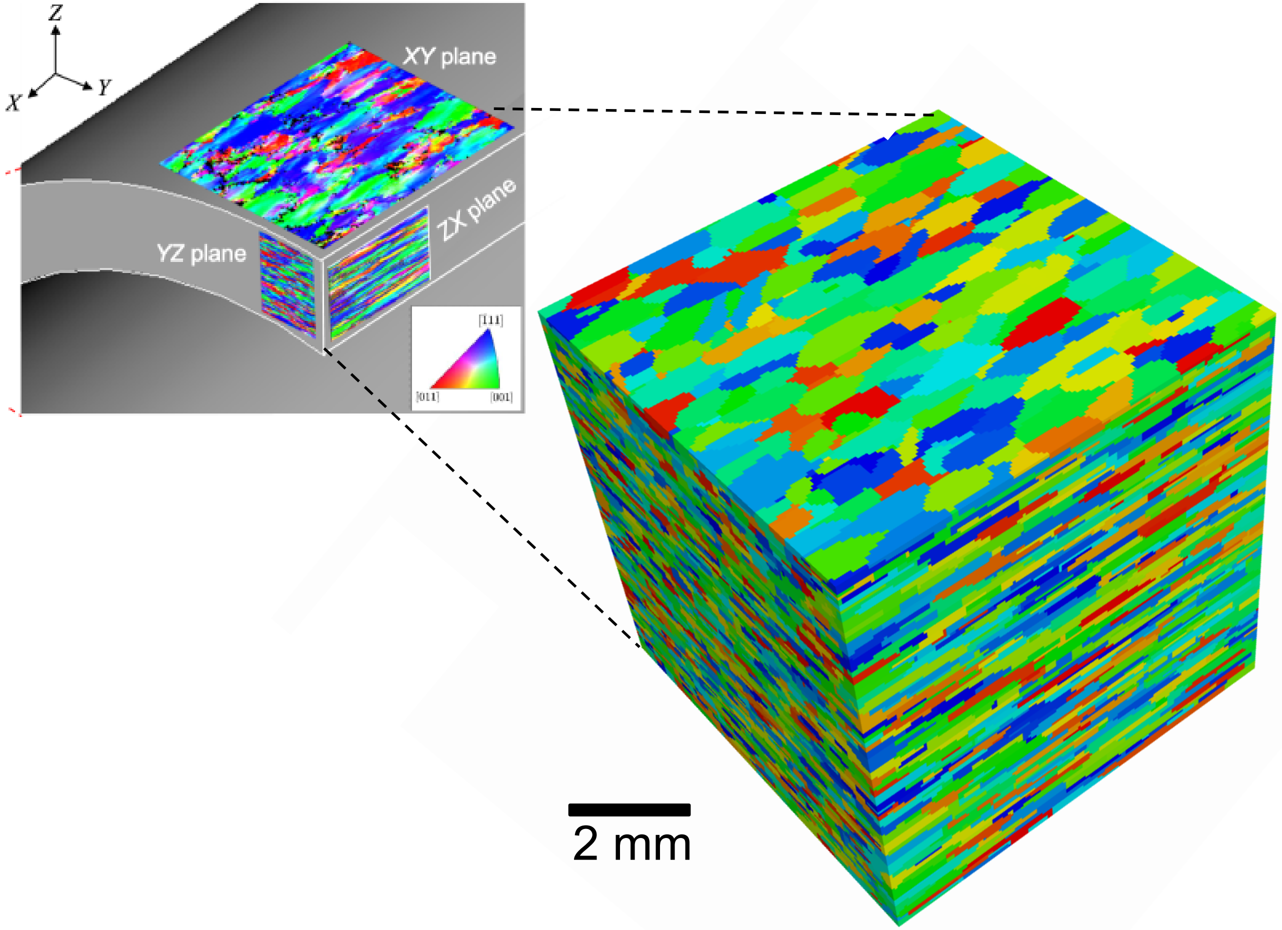
- Grain-level (mesoscale) approach to materials modeling using multiscale strategies – realistic length and time scales
- Explicitly model discrete grains and slip systems based on dislocation slip
- Predicts heterogeneous material's responses resulting from microstructure.
- More predictive than macroscopic plasticity models (e.g. texture evolution and elastic/plastic anisotropy)

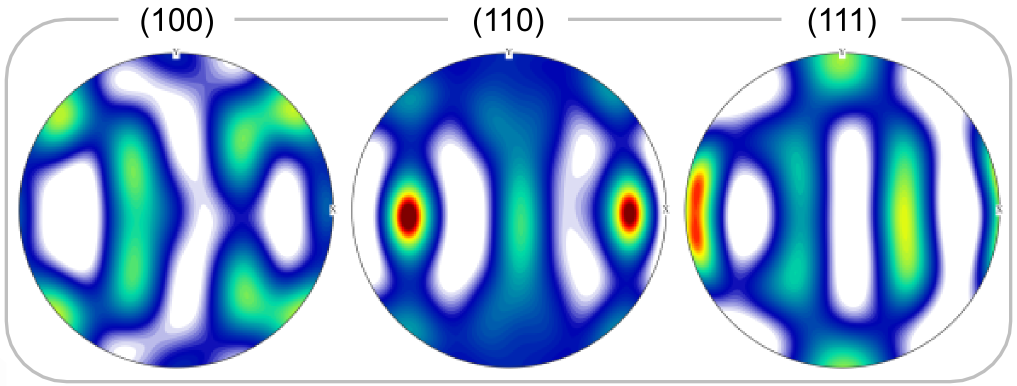
- *Slip rate:* $\dot{\gamma}^\alpha = \dot{\gamma}^0 \left(\frac{\tau^\alpha}{g^\alpha}\right)^{1/m}$
- *Slip resistance:* $g^\alpha = g_0 + A\mu b \sqrt{\sum_{\beta=1}^{12} H^{\alpha\beta}\rho^\beta}$
- *Dislocation evolution:*

$$d\rho^\alpha = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{12} \rho^\beta} - \kappa_2 \rho^\alpha\right) |d\gamma|$$

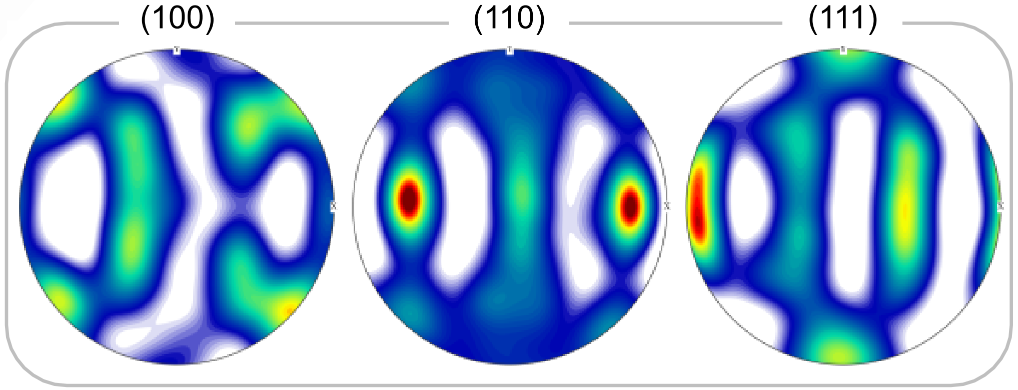
- *Hardening matrix:* $H^{\alpha\beta} = \mathbf{n}^\alpha \cdot \xi^\beta$
- *12 {111}<110> slip systems for FCC*

Computational microstructures 1: Sampled texture





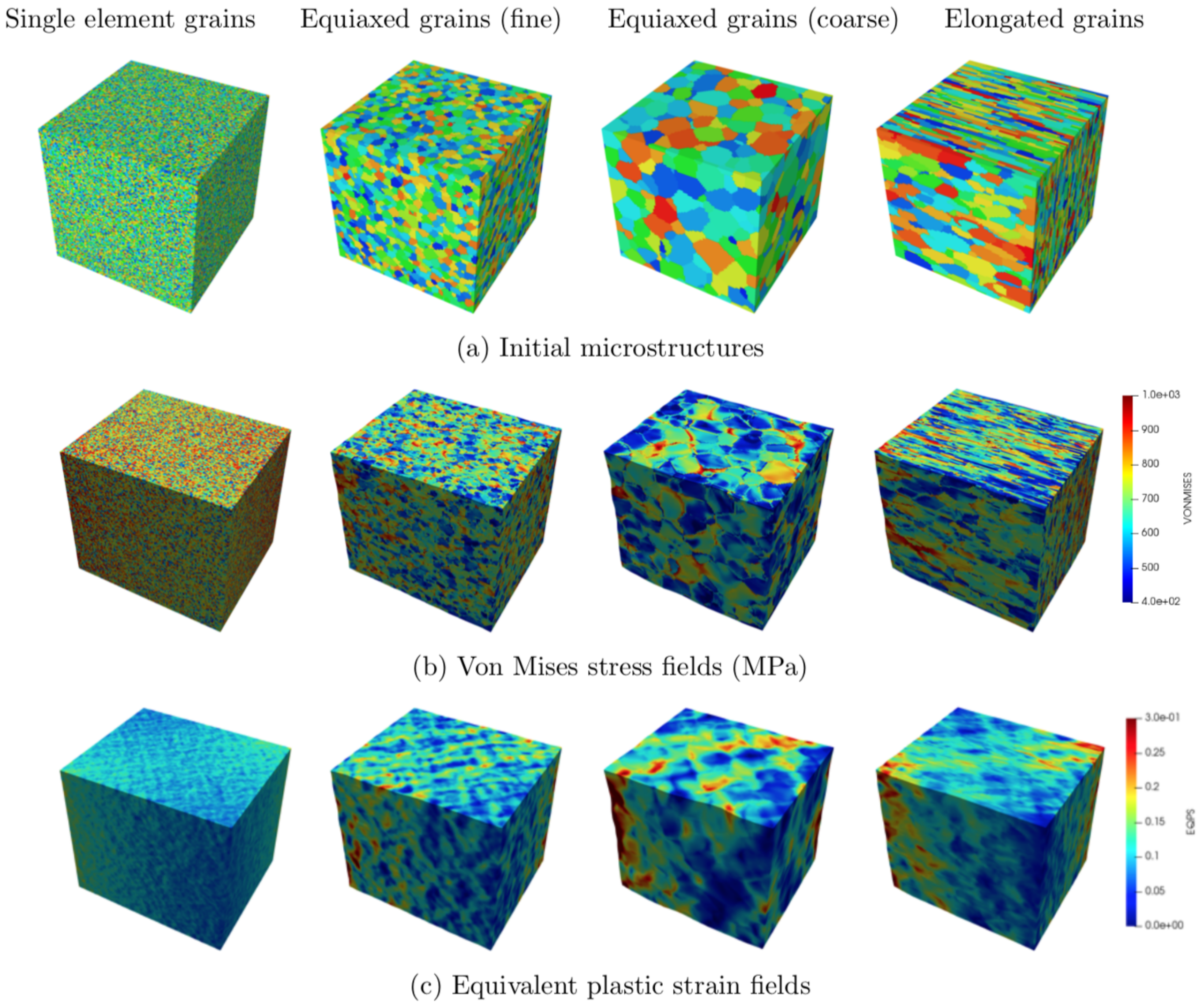
XRD (10^6 data points)

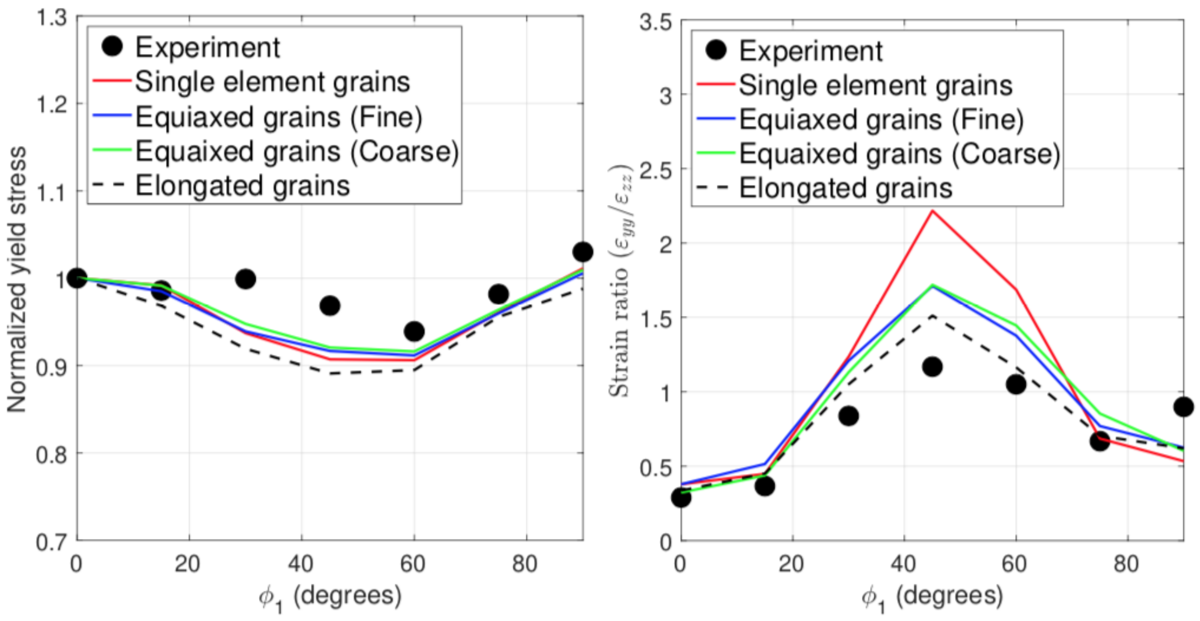


"Sampled texture"

FE mesh: 3,375,000 (150×150×150) hex elements
Average grain aspect ratio ~ 7:3:1 along X, Y, Z directions
RVE with ~3,000 grains

Effects of initial microstructures





CP-FE simulations

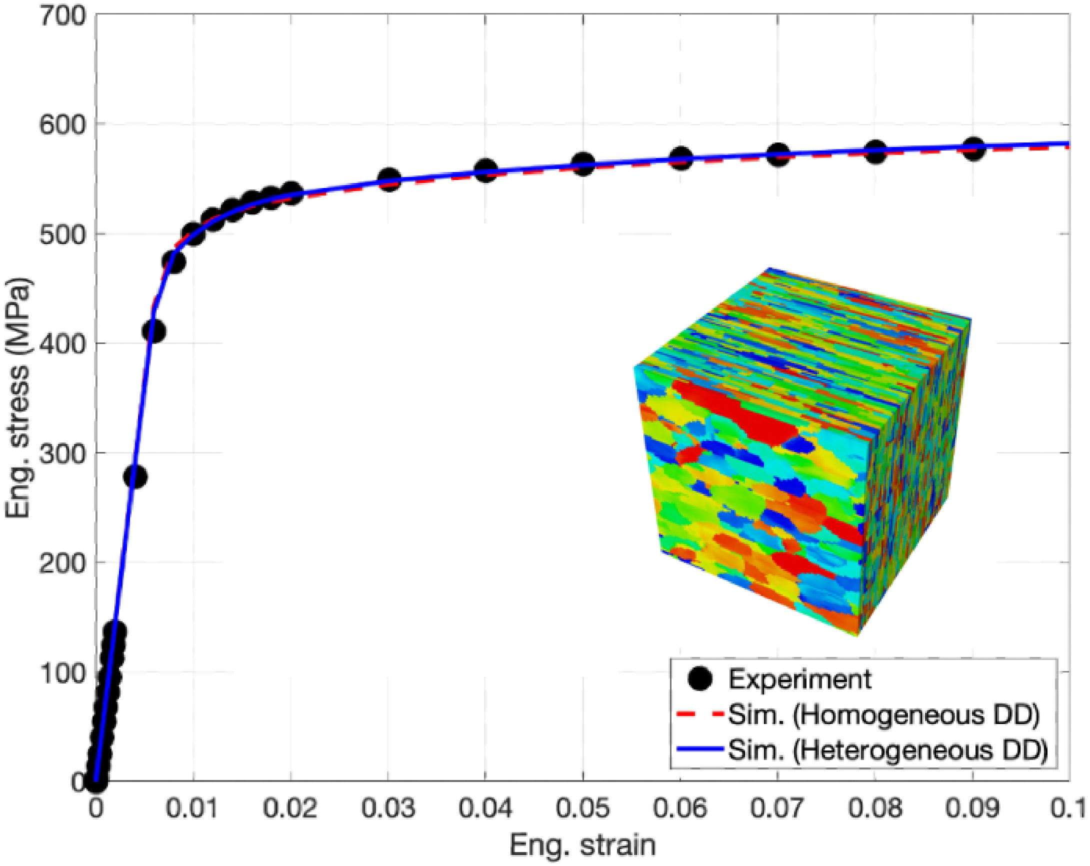
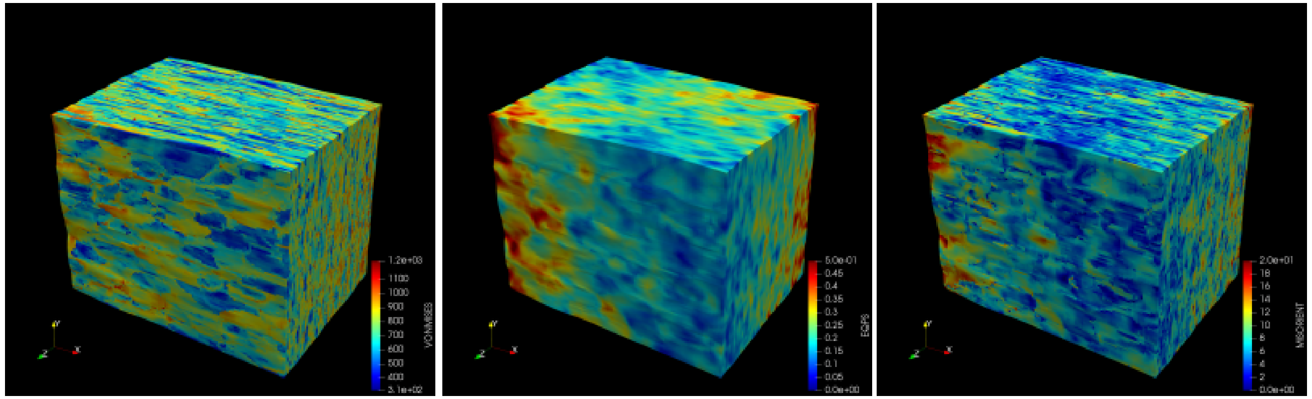


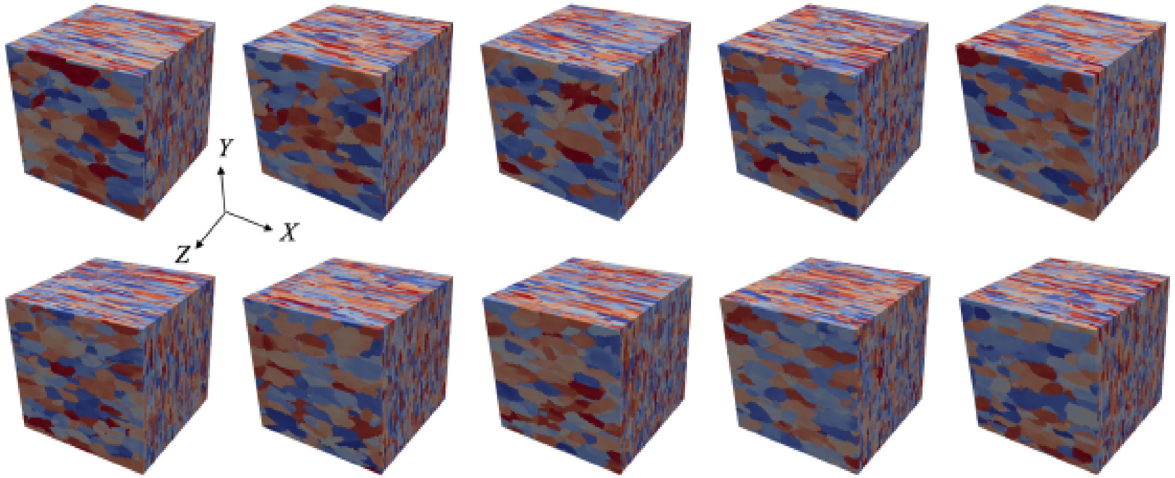
Table 2. Material parameters used in the sampled texture CP-FEM simulations.

Constants	Values	Constants	Values	Constants	Values
C_{11}	108.2 GPa	$\dot{\gamma}_0$	10^{-5} s^{-1}	ρ_0	1.17×10^{14} m^{-2}
C_{12}	61.3 GPa	m	0.012	κ_1	4.0×10^{8} m^{-1}
C_{44}	28.5 GPa	A	0.4	κ_2	28
μ	25.7 GPa	b	2.86×10^{-10} m	g_0	143 MPa



Von Mises stress | Equivalent plastic strain | Crystal rotations

Deformed microstructures at 20%



10 realizations of equivalent microstructures