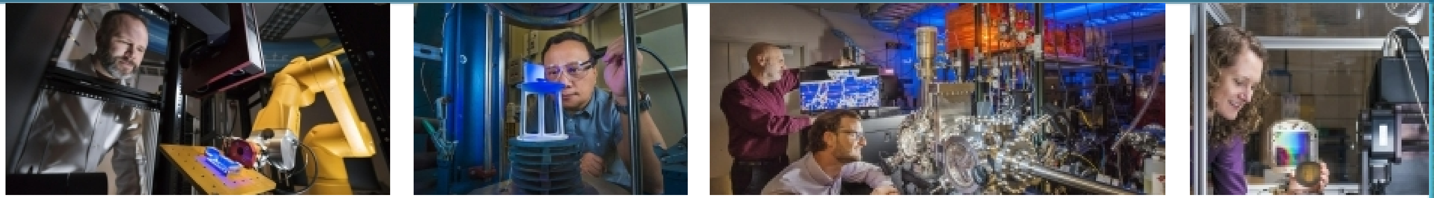
SAND2022-5849C

Sandia National Laboratories

Predicting plastic anisotropy using crystal plasticity and Bayesian neural network surrogate models



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Materials Science & Engineering

M S R F

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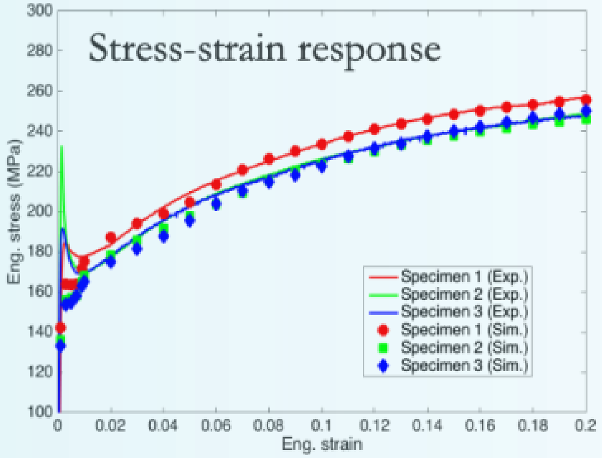
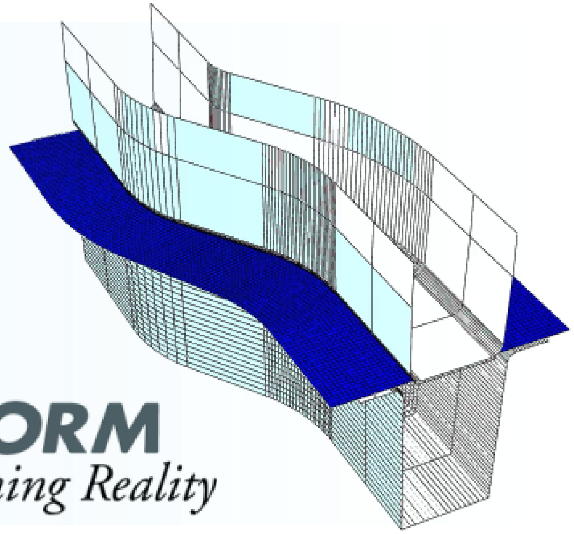
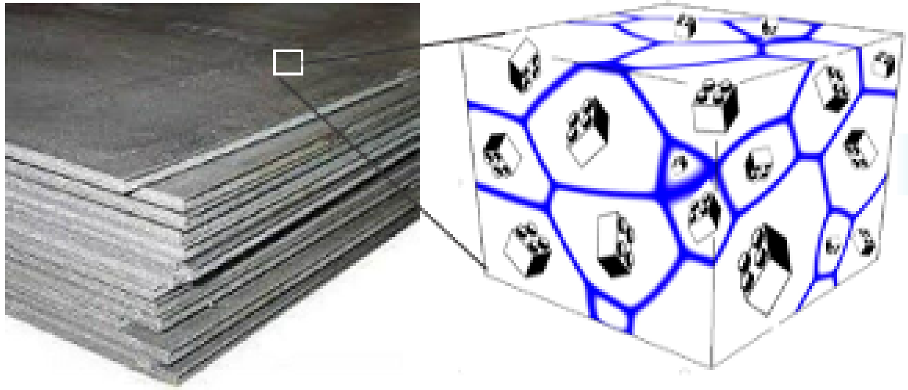
Structure-Property: Traditional Paradigm

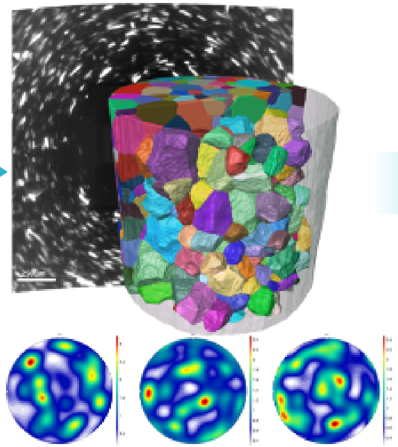


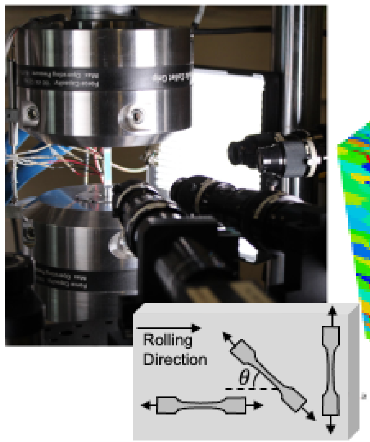
AUTOFORM
Forming Reality

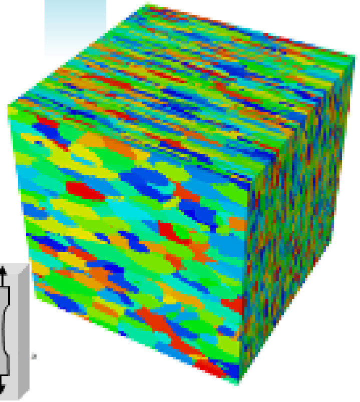


Calibrated Model Parameters
(e.g., Hill's quadratic anisotropic yield model constants)

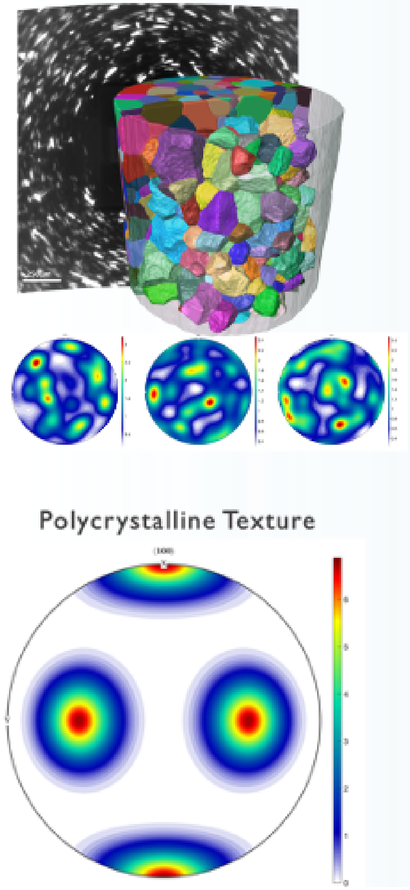


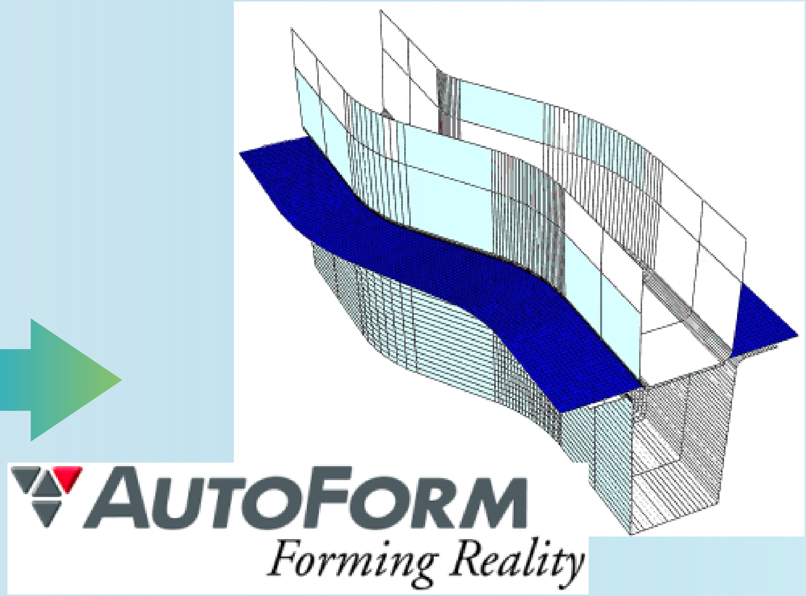






Structure-Property: Agile, Data-driven Paradigm

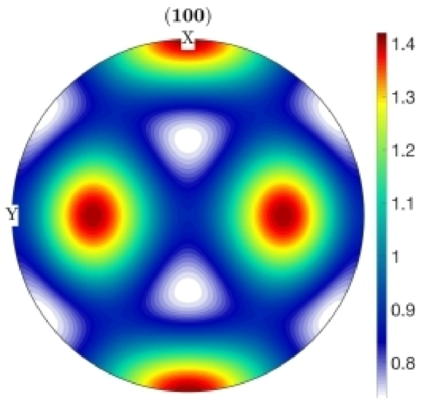


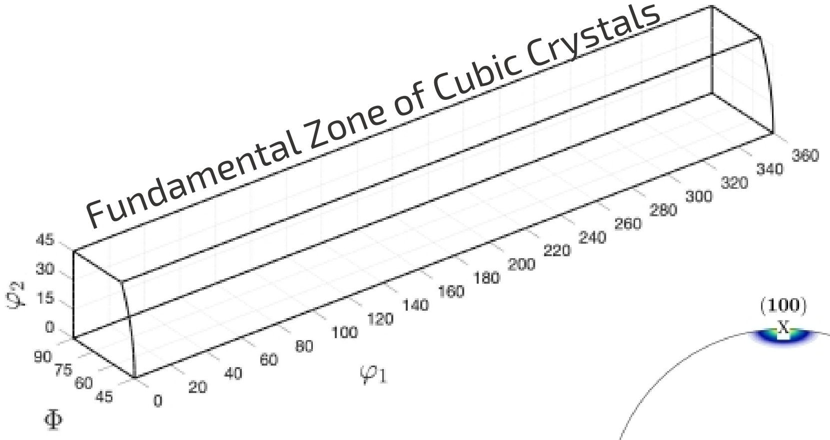


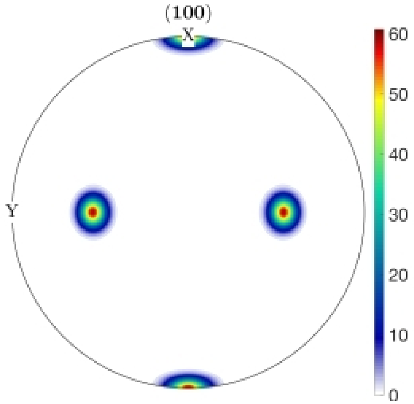
Calibrated Model Parameters
(e.g., Hill's quadratic anisotropic yield model constants)

Surrogate Model: Generation of Dataset

Pole figure with spread of 35 °

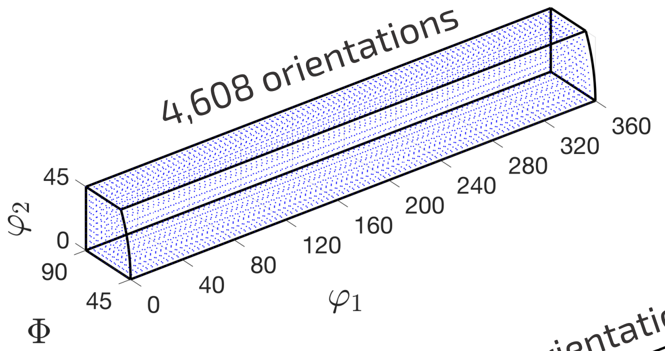




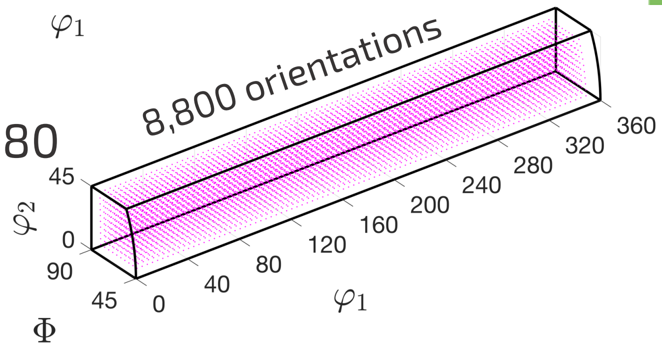


Pole figure with spread of 5 °

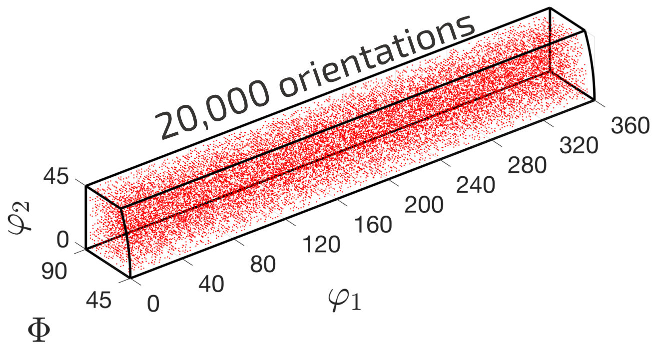
Apply 9 levels of spread every 5° from 0 ° to 45 °



Training Textures: 54,480



Testing Textures: 20,00



Apply random spread between 1 ° and 50 °

Perform crystal plasticity to calibrate Hill's Constants for each texture

$$\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha=1}^{12} \dot{\gamma}^\alpha \mathbf{s_0}^\alpha \otimes \mathbf{n_0}^\alpha$$

$$F = \frac{1}{2}\left[-\left(\frac{\sigma_0}{\sigma_{xx}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{yy}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{zz}}\right)^2\right]$$

$$G = \frac{1}{2}\left[\left(\frac{\sigma_0}{\sigma_{xx}}\right)^2 - \left(\frac{\sigma_0}{\sigma_{yy}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{zz}}\right)^2\right]$$

$$H = \frac{1}{2}\left[\left(\frac{\sigma_0}{\sigma_{xx}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{yy}}\right)^2 - \left(\frac{\sigma_0}{\sigma_{zz}}\right)^2\right]$$

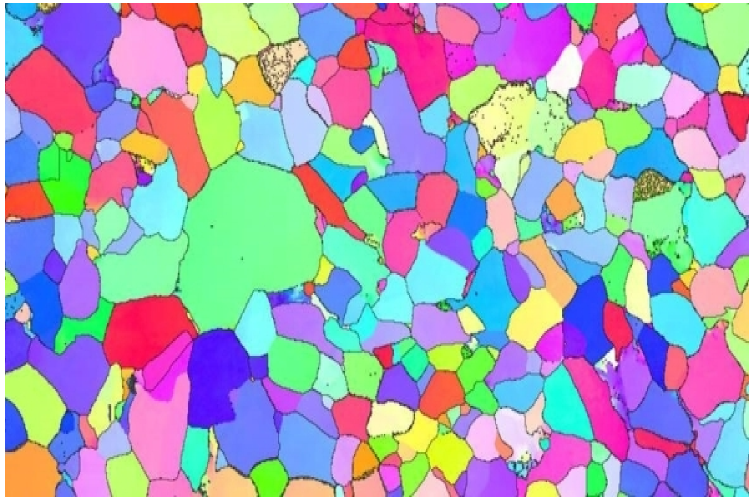
$$L = \frac{1}{2}\left[\left(\frac{2\sigma_0}{\sigma_{yz}}\right)^2 - G - H\right]$$

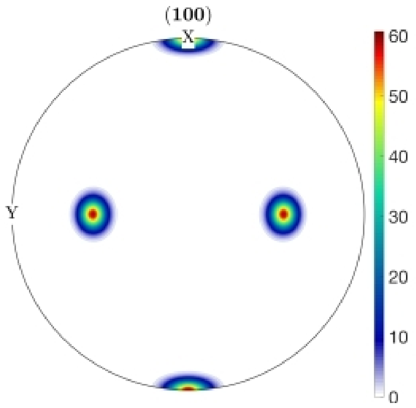
$$M = \frac{1}{2}\left[\left(\frac{2\sigma_0}{\sigma_{zx}}\right)^2 - H - F\right]$$

$$N = \frac{1}{2}\left[\left(\frac{2\sigma_0}{\sigma_{xy}}\right)^2 - F - G\right]$$

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.

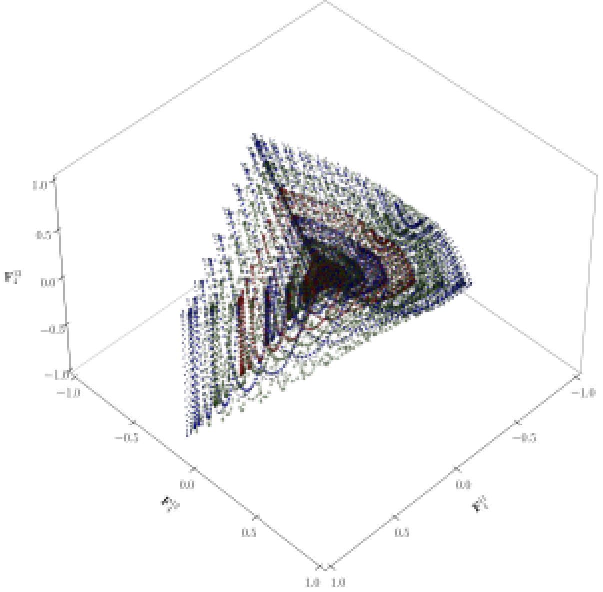
Fourier Series Representation:

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

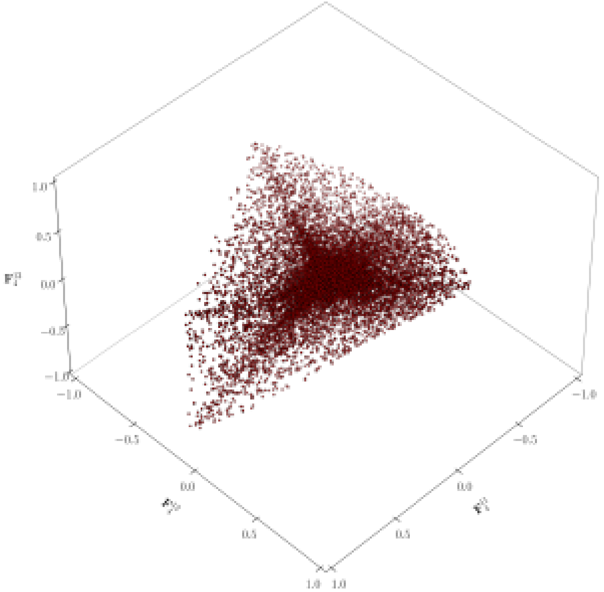
$$f_s(g) = \sum_{\mu,n,l} F_{ls}^{\mu n} T_l^{\mu n}(g),$$

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

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

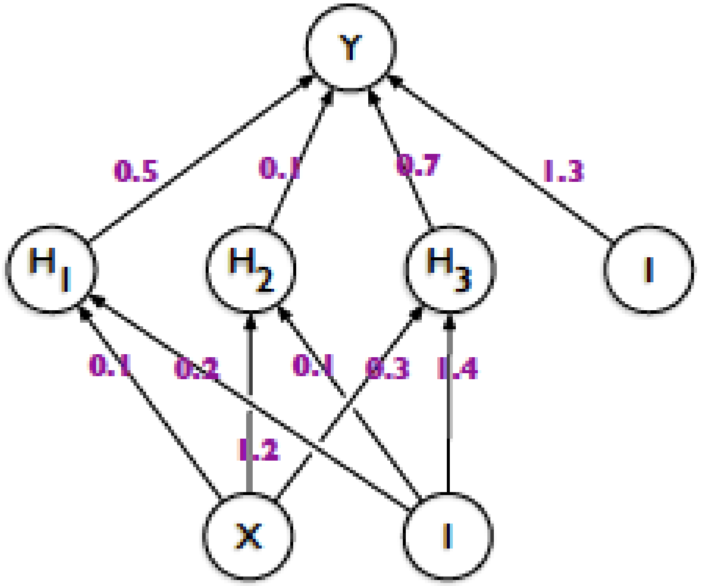


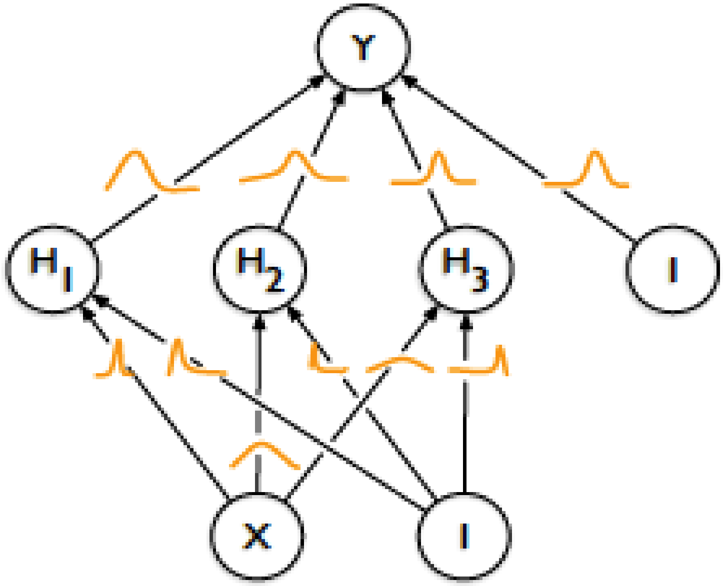
GSH representation of Training Textures



GSH representation of Testing Textures

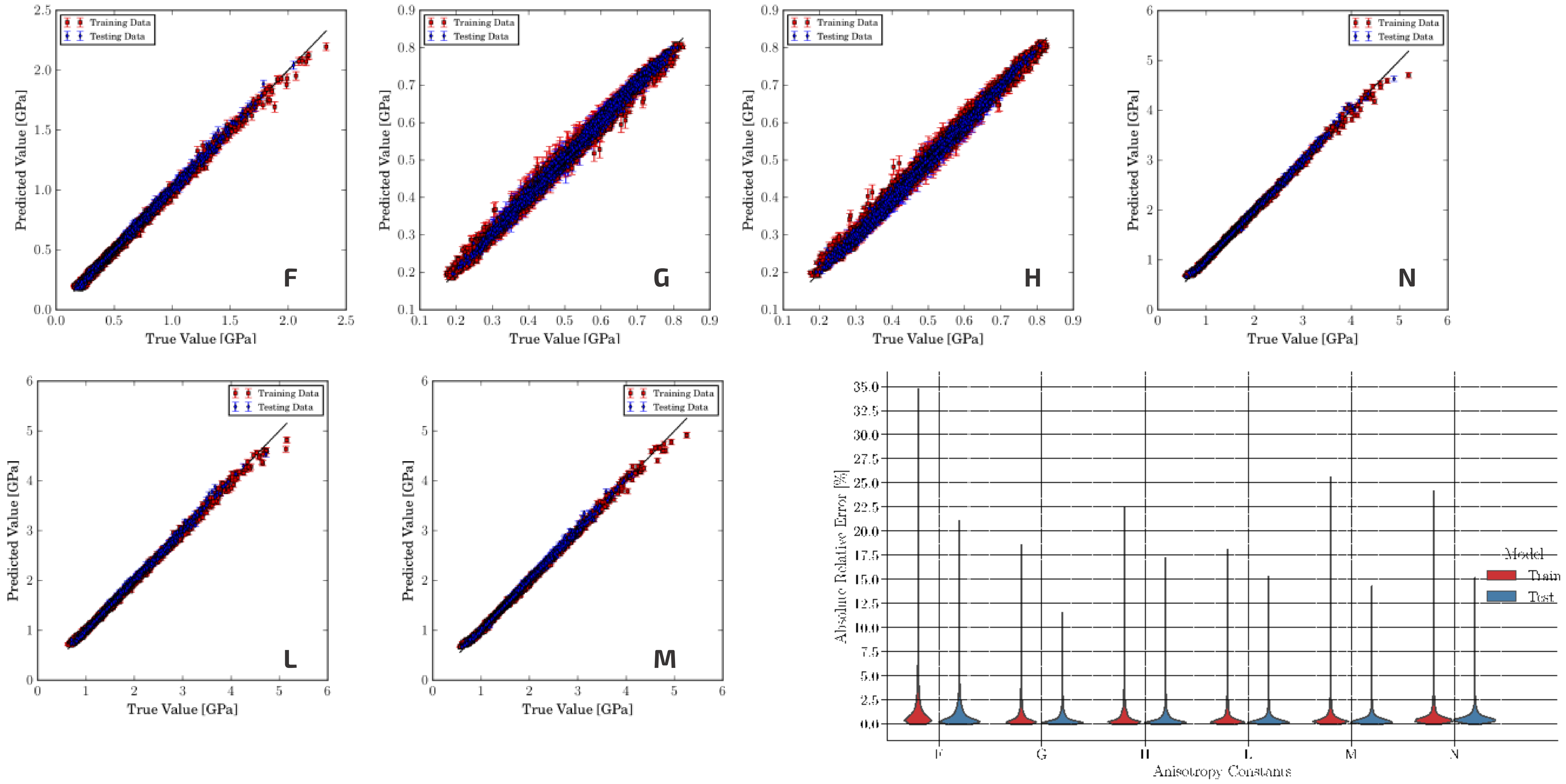
Surrogate Model: Neural Network Linkage





- Monte Carlo Sampling of 50 steps to sample the distribution of weights to obtain a distribution of values.
- Architecture of 2 hidden layers with 81 nodes on each layer and sigmoid activation function to predict the output.
- Architecture trained to 5000 epochs.

Surrogate Model: Validating the developed Model

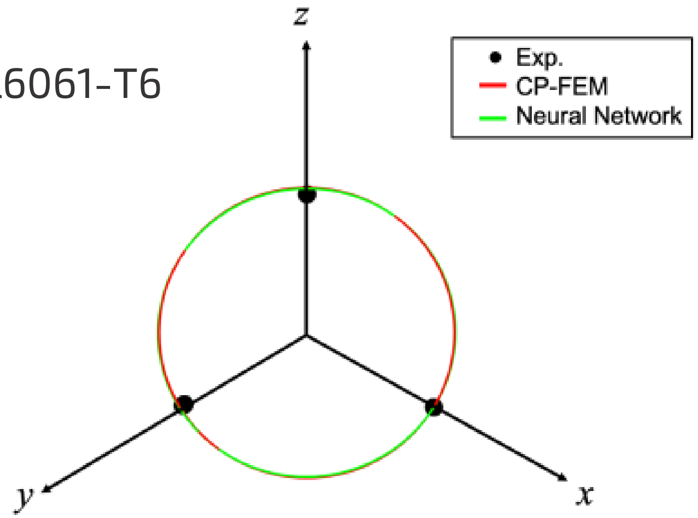


Surrogate Model: Experimental Validation

Parameterizing Hill's quadratic anisotropic yield model:

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

Al6061-T6

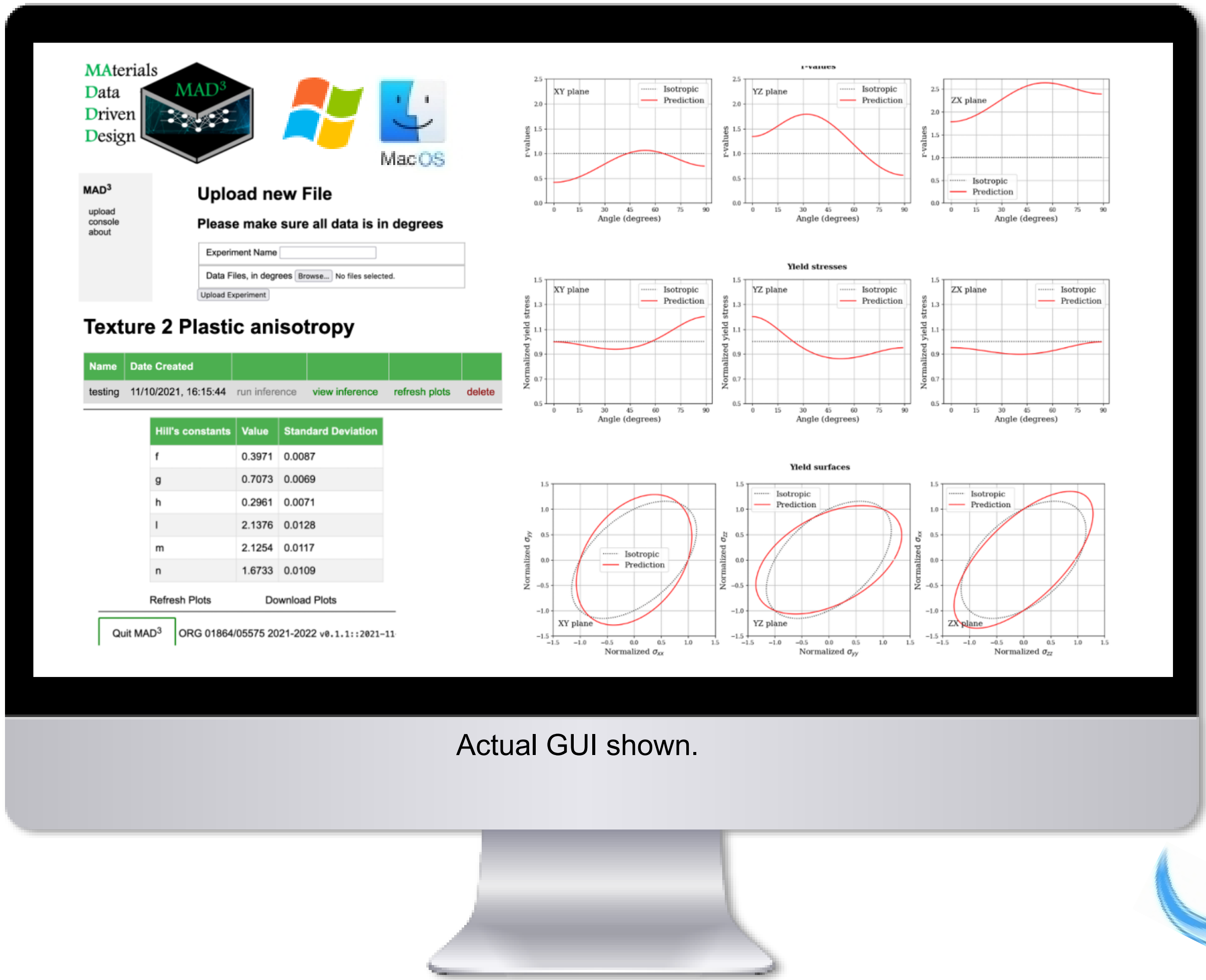


π-plane yield surfaces of Al6061

Al6061-T6	F	G	H	L	M	N	TIME
Experiments	0.6097	0.5495	0.4061	-	-	-	3-6 months
Crystal plasticity-FE	0.5268	0.5261	0.4739	1.5258	1.4788	1.7604	~10 h in HPC
Neural Network predictions	0.5298 ±0.0013	0.5369 ±0.0010	0.4631 ±0.0010	1.5735 ±0.0017	1.5296 ±0.0013	1.6548 ±0.0015	<1 sec.

Obtain Parameterized Constants 36000 times faster than Crystal Plasticity.

Surrogate Model: GUI-based Software Solution



Actual GUI shown.

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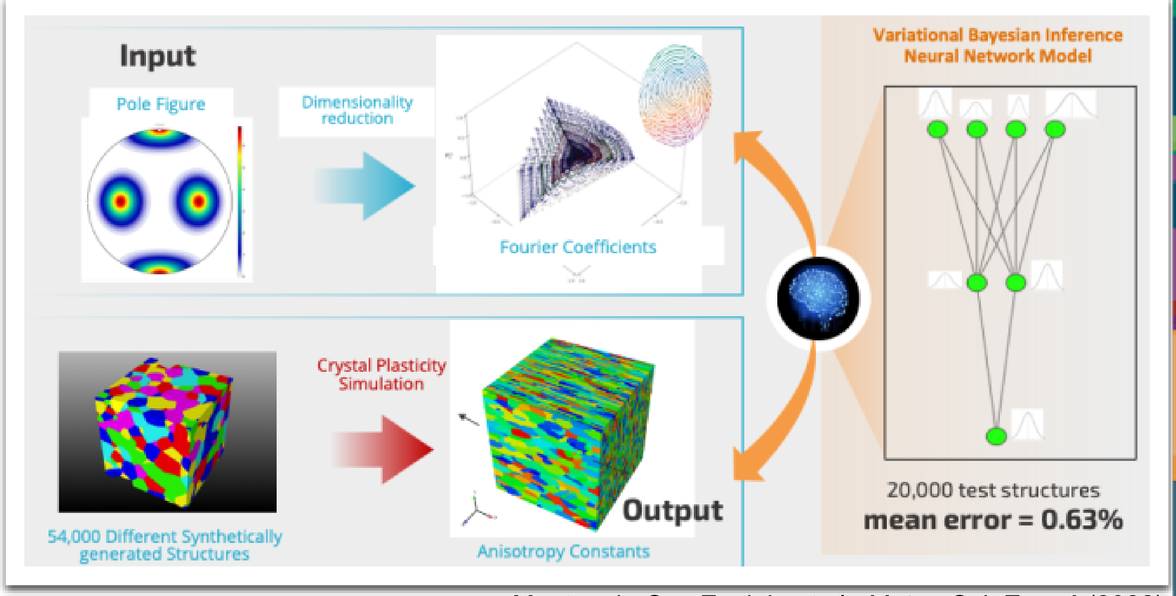
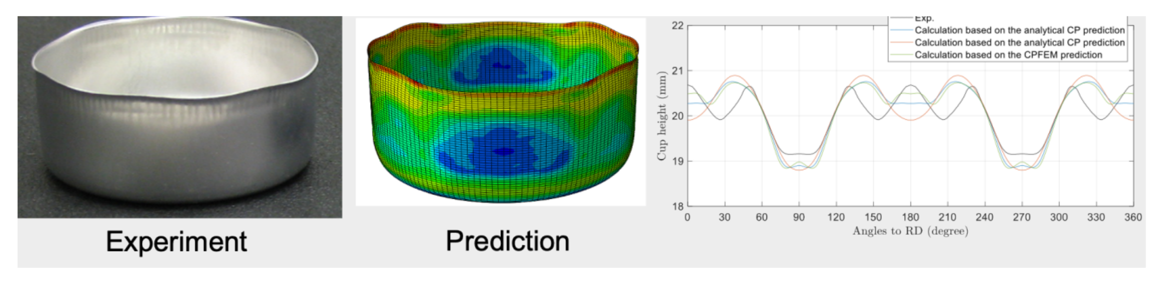
Theory: Machine Learning based anisotropy prediction



Montes de Oca Zapiain et al., *Mater. Sci. Eng. A* (2022)

Application (e.g., metal forming analysis)



Structure-Property: Conclusion

- Deep learning enabled us to establish an accurate and computationally efficient linkage between the underlying internal structure of the material and the resultant desired anisotropic constants while accounting for the uncertainty.

Questions?

Generalized Spherical Harmonics

GSH Representation of Texture

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

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

GSH Representation of Single Crystal Texture

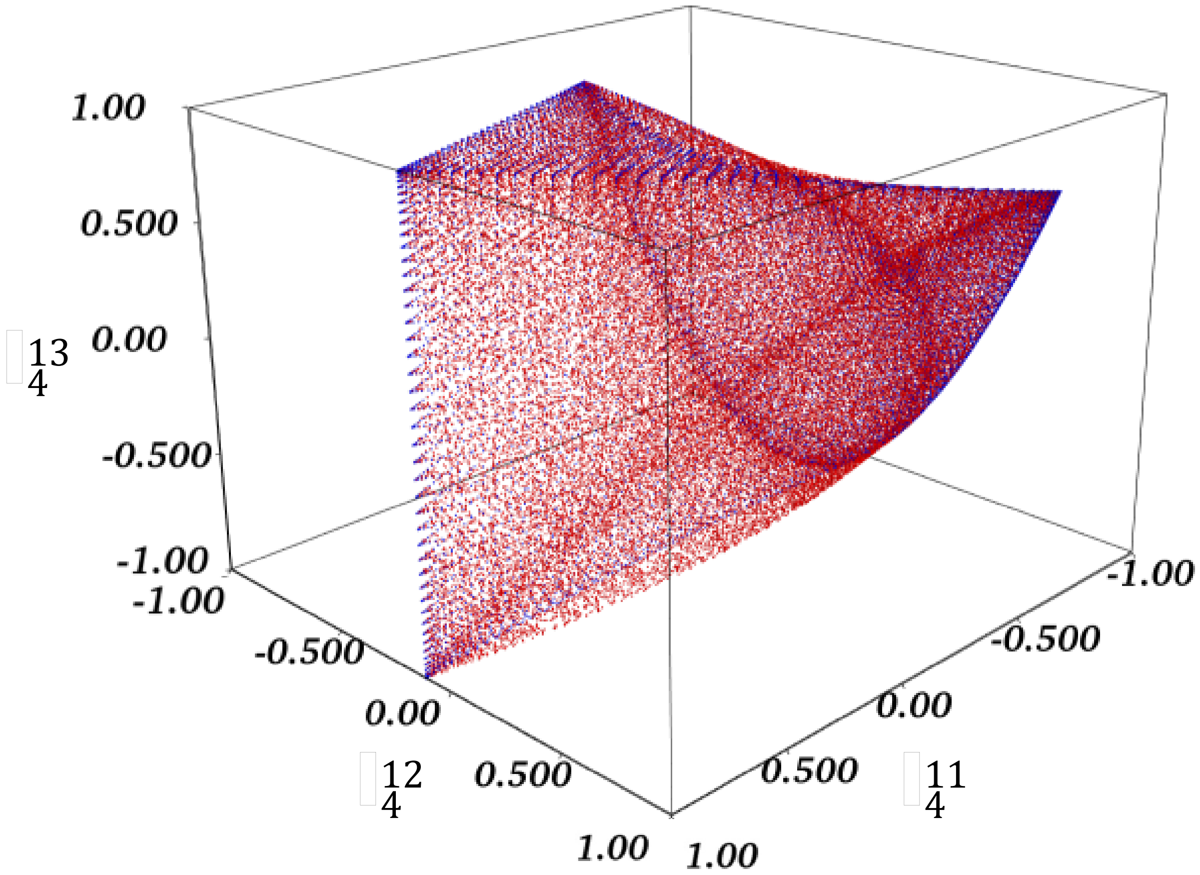
$$f(g) = \delta(g - g_0) = \sum_{\mu,n,l} F_l^{\mu n} T_l^{*\mu n}(g)$$

GSH Representation of Polycrystalline Texture

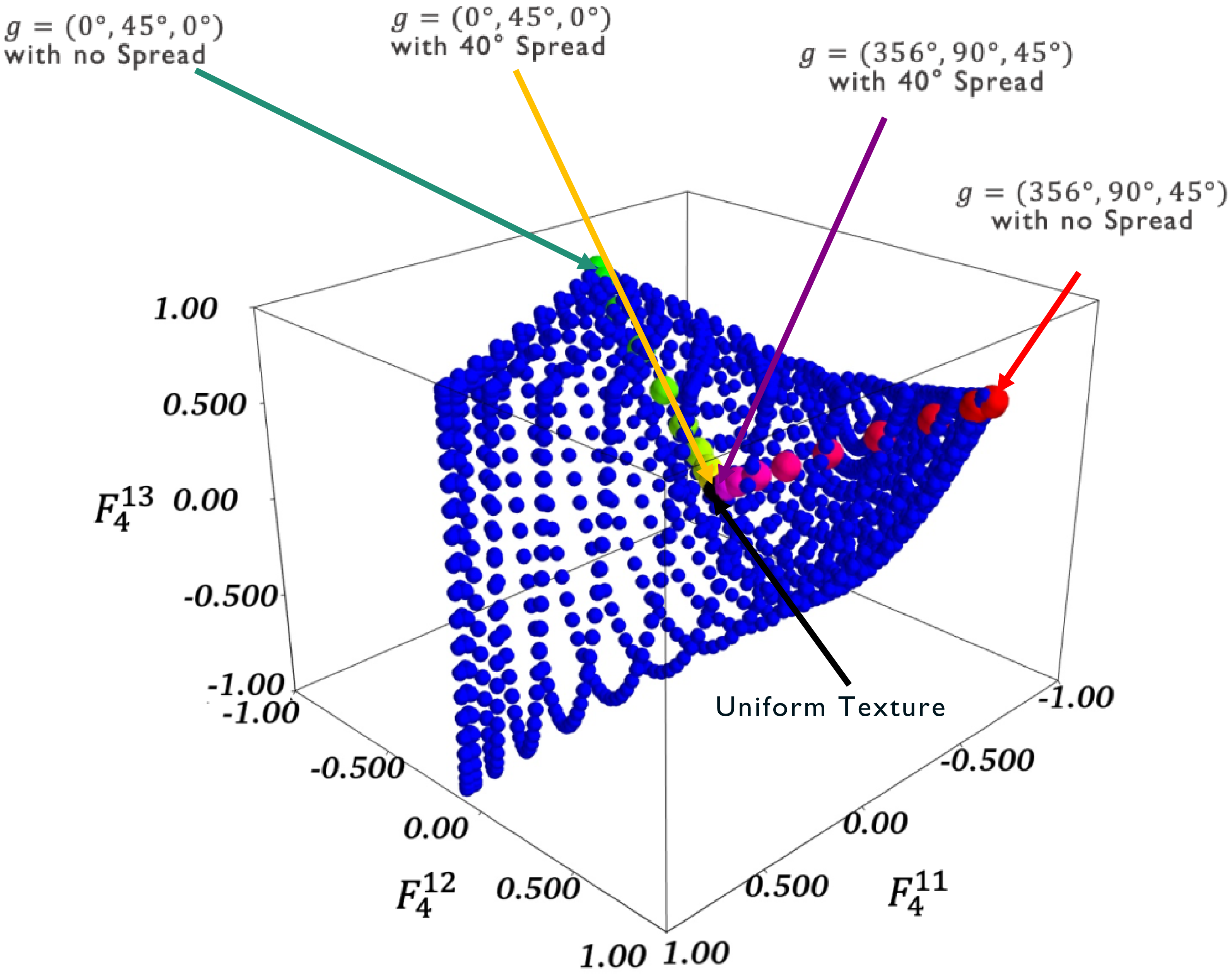
$$F_{polycrystal}{}_l^{\mu n} = \sum_j w_j \; F_{l,j}^{\mu n}$$

Volume fraction

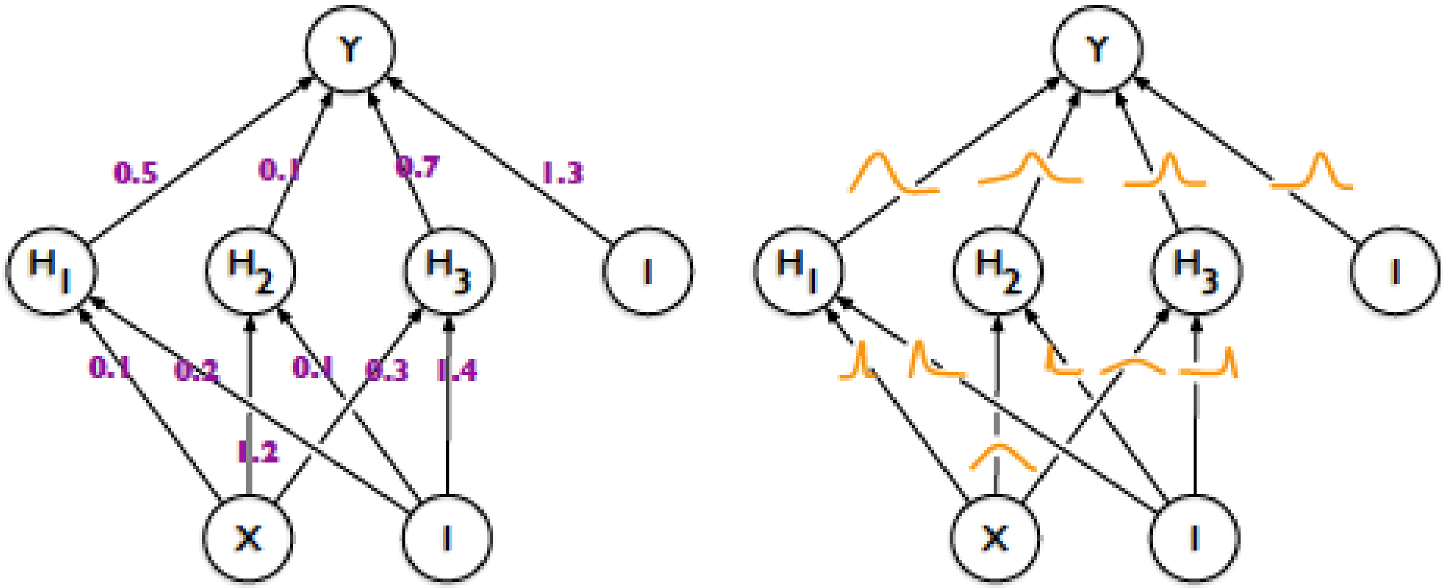
GSH Representation of all Possible Orientations in the Cubic FZ



GSH Representation



Machine Learning Surrogate Model



- Bayesian Neural Network that trains the parameters that describe the distribution of the weights and biases.
- Uses Monte Carlo Sampling (50 steps) to sample the distribution of weights to obtain a distribution of values.
- Enables the incorporation of uncertainty in the prediction.
- Architecture of 2 hidden layers to predict the output.