Program in Applied Mathematics

CVPR
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Learning microstructure–property relationships in materials with robust features from vision transformers

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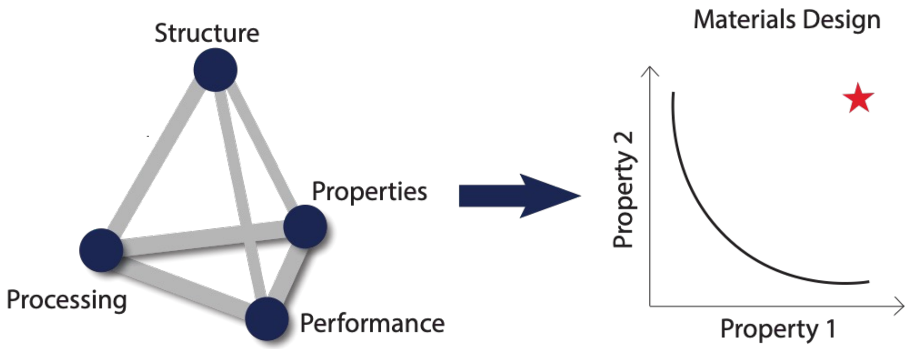
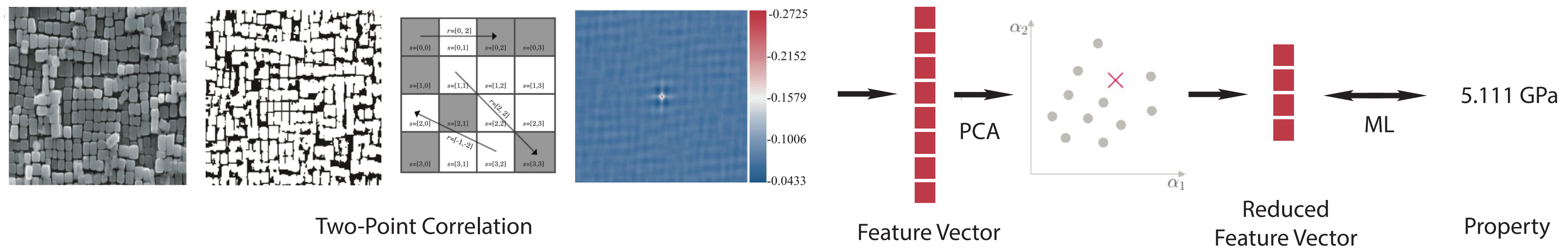
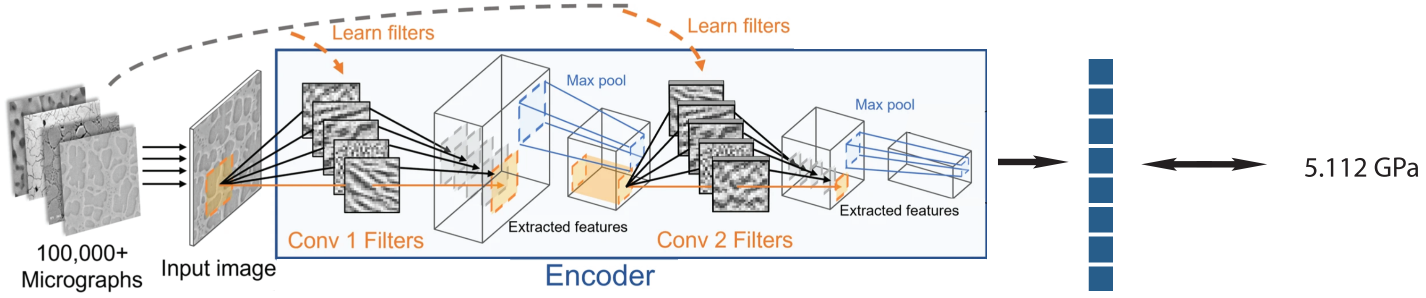
Microstructure-Property Relationships



- Design of structural alloys relies on quantitative understanding of microstructure–property relationships.
- Machine learning can be used to accelerate the design process.
- Quantitative descriptions of microstructures are needed to utilize machine learning.

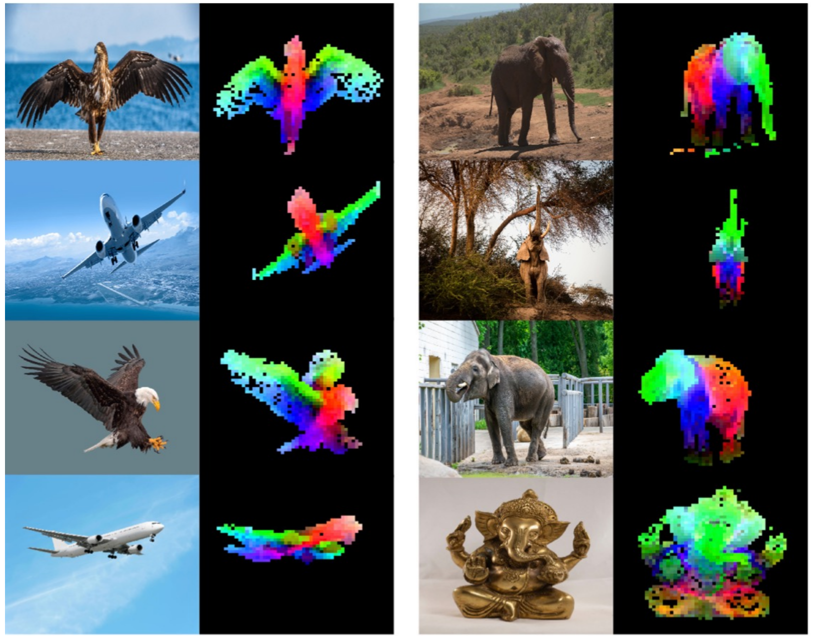


Two-Point Correlation

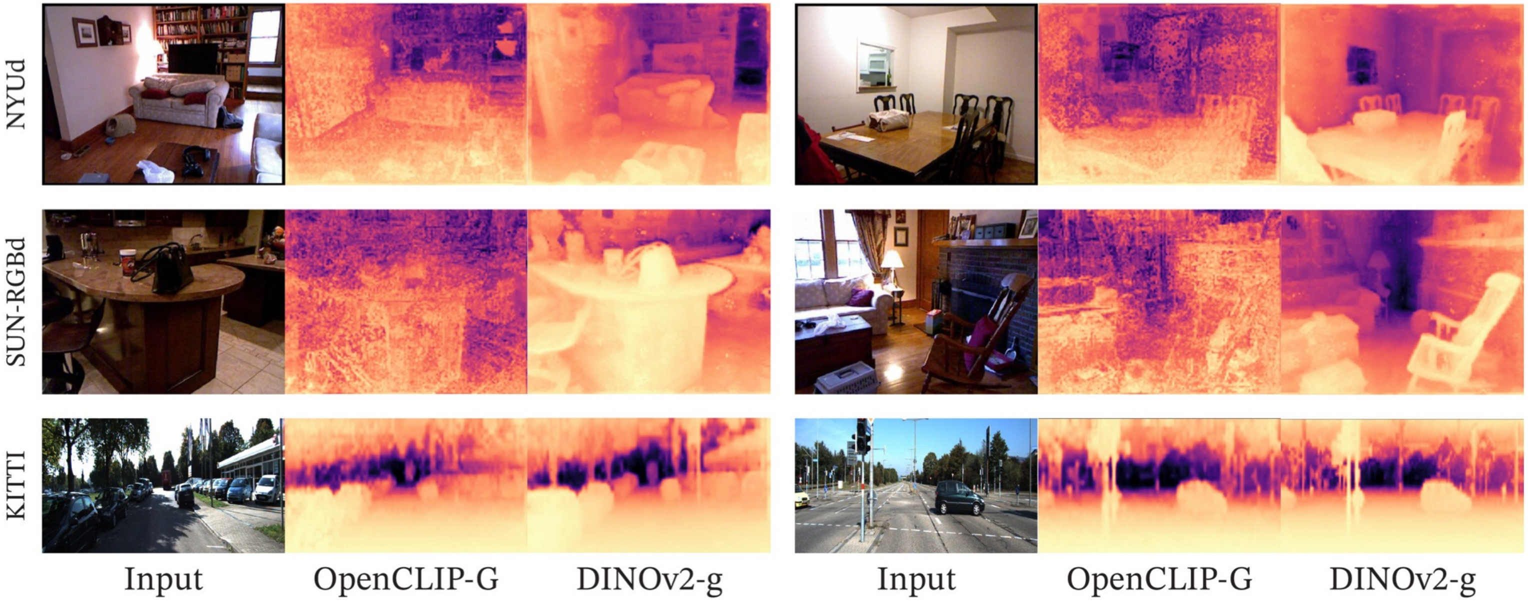


Convolutional Neural Network Latent Representation

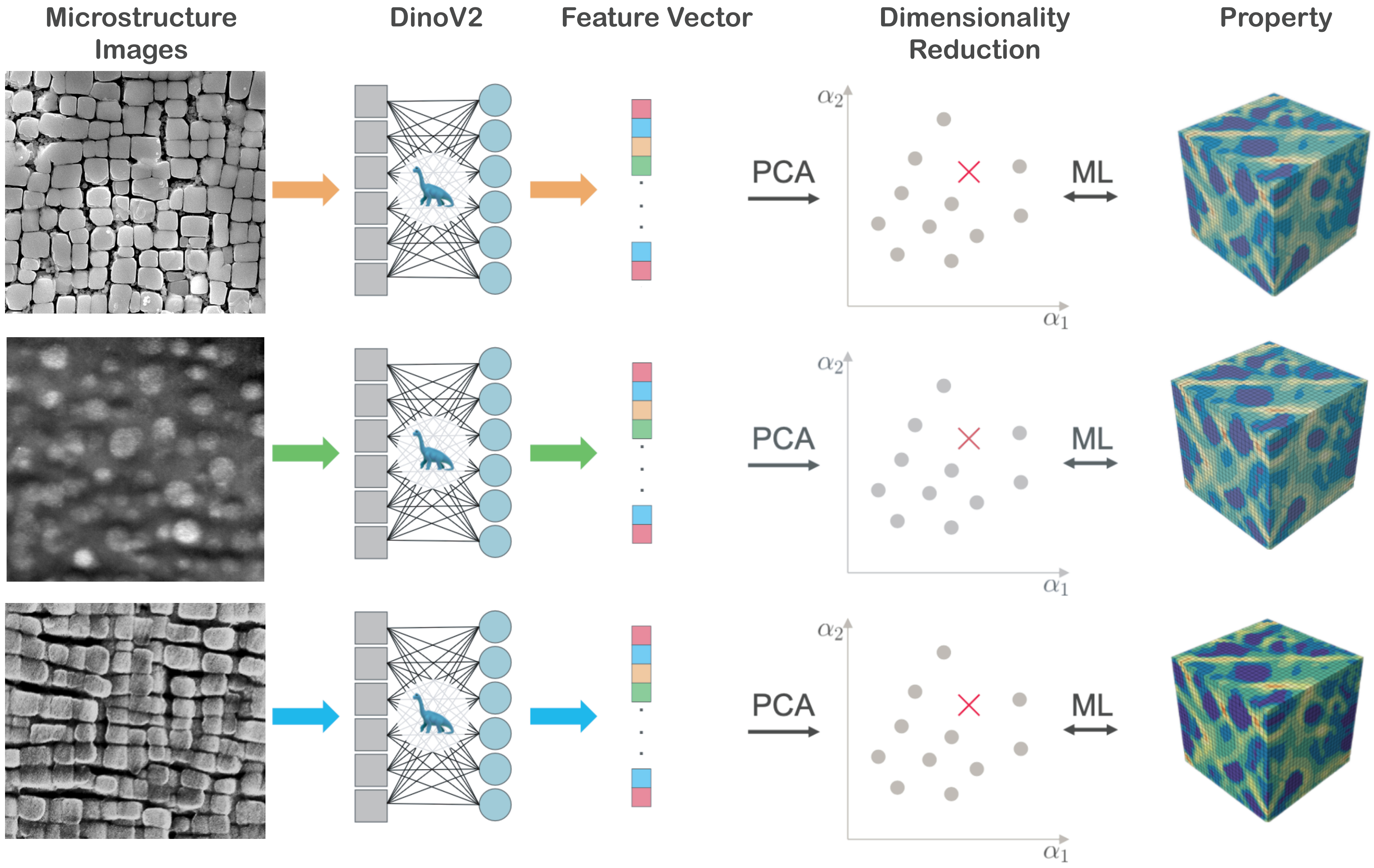
DinoV2



Method	Arch.	NYUd (0.330)			KITTI (2.10)			NYUd → SUN RGB-D (0.421)		
		lin. 1	lin. 4	DPT	lin. 1	lin. 4	DPT	lin. 1	lin. 4	DPT
OpenCLIP	ViT-G/14	0.541	0.510	0.414	3.57	3.21	2.56	0.537	0.476	0.408
MAE	ViT-H/14	0.517	0.483	0.415	3.66	3.26	2.59	0.545	0.523	0.506
DINO	ViT-B/8	0.555	0.539	0.492	3.81	3.56	2.74	0.553	0.541	0.520
iBOT	ViT-L/16	0.417	0.387	0.358	3.31	3.07	2.55	0.447	0.435	0.426
DINOv2	ViT-S/14	0.449	0.417	0.356	3.10	2.86	2.34	0.477	0.431	0.409
	ViT-B/14	0.399	0.362	0.317	2.90	2.59	2.23	0.448	0.400	0.377
	ViT-L/14	0.384	0.333	0.293	2.78	2.50	2.14	0.429	0.396	0.360
	ViT-g/14	**0.344**	**0.298**	**0.279**	**2.62**	**2.35**	**2.11**	**0.402**	**0.362**	**0.338**



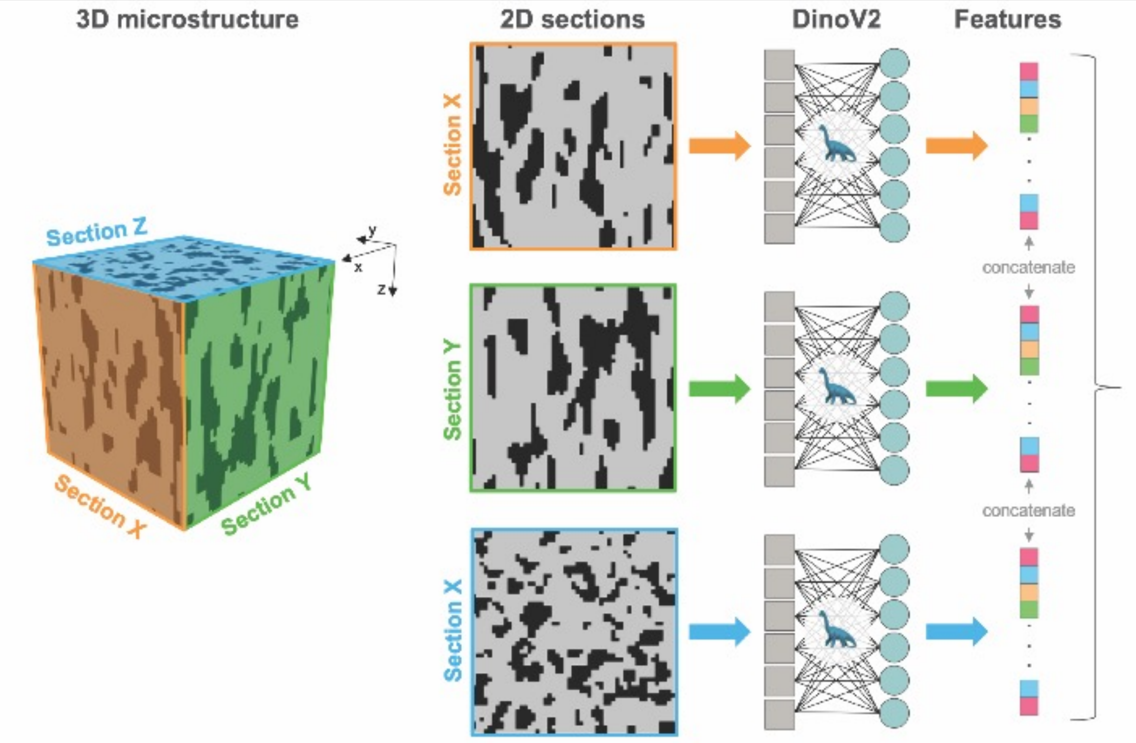
Methodology

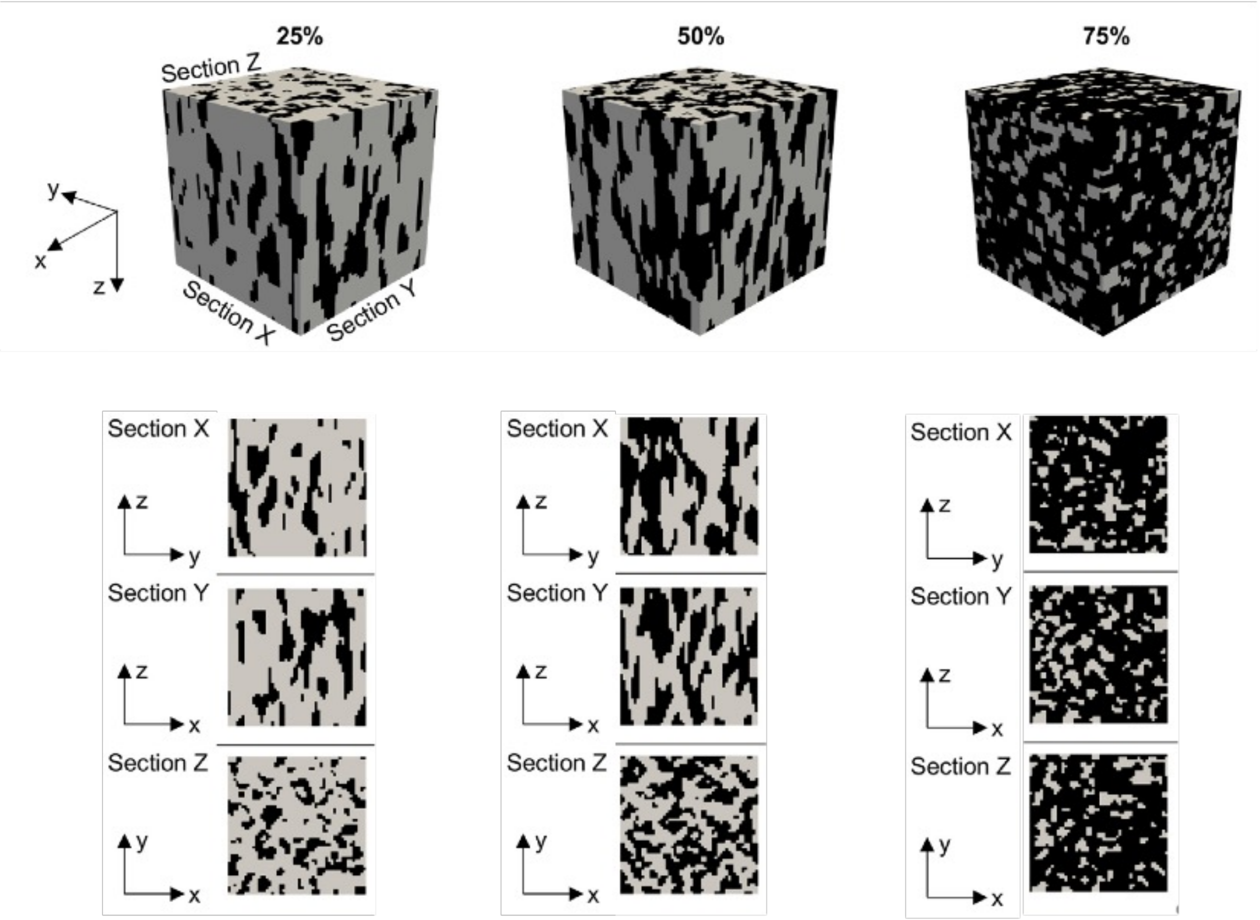


Peng et al. 2018. Picasso et al. 2008. Zhang et al. 2018.

Case Study 1 – Young’s modulus from simulations

5900 x 3 slices of simulated microstructures*
and their corresponding Young’s moduli



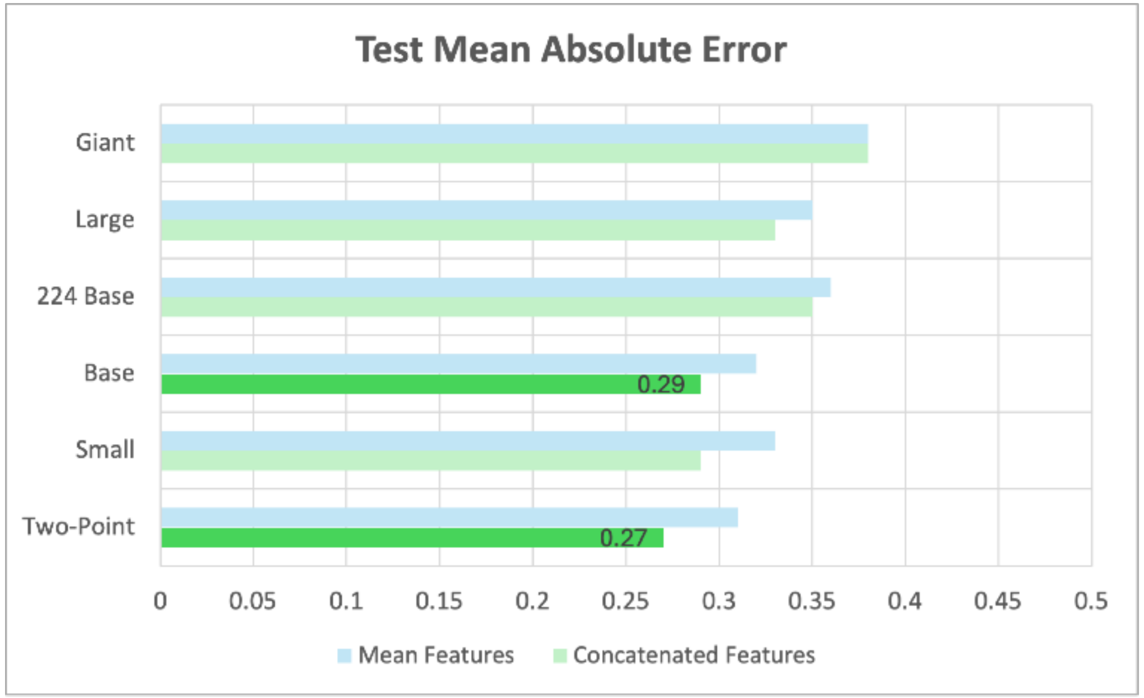


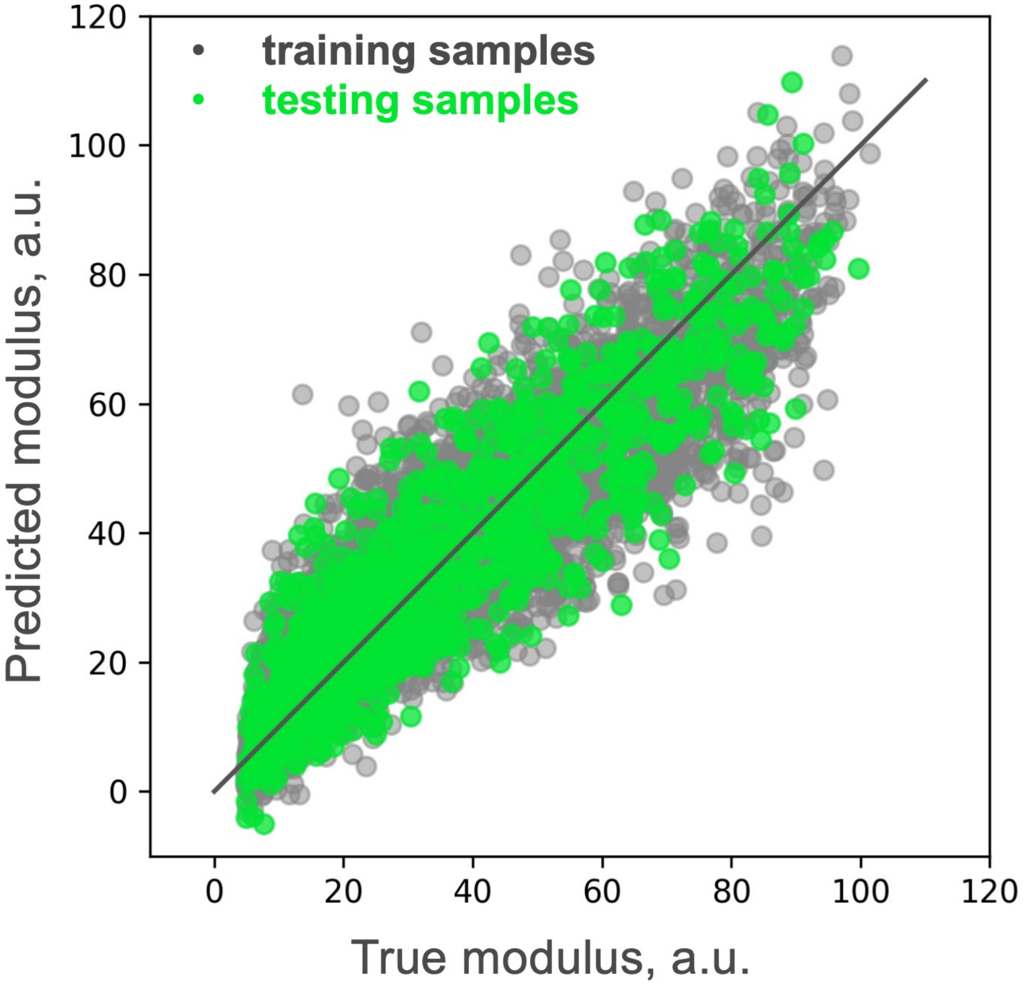
Feature aggregation from 2D sections:

- concatentation
- mean pooling

Case Study 1: Results

- The best DinoV2 model is the base model with 17 principal components of concatenated (3 · 768) features.



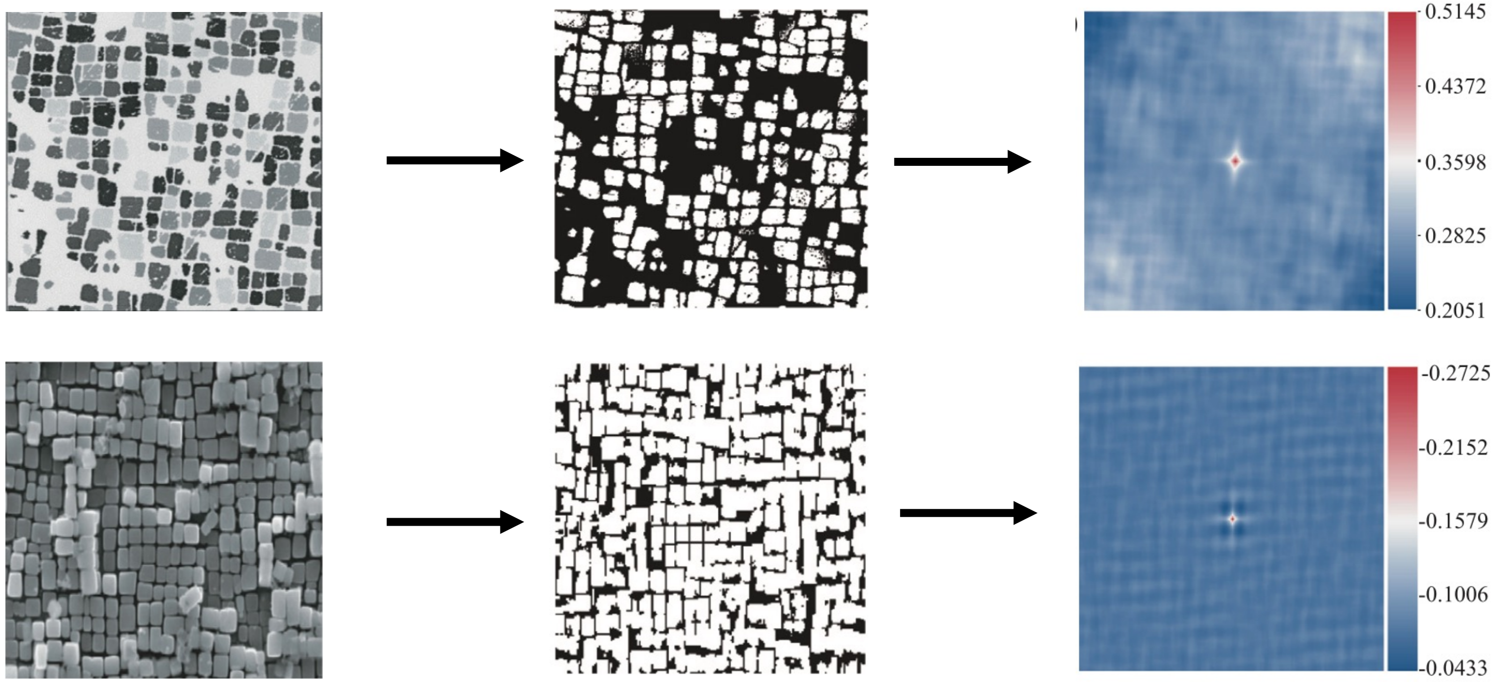


Parity plot showing the prediction results of the base DinoV2 model.

Digital Data vs. Experimental Data

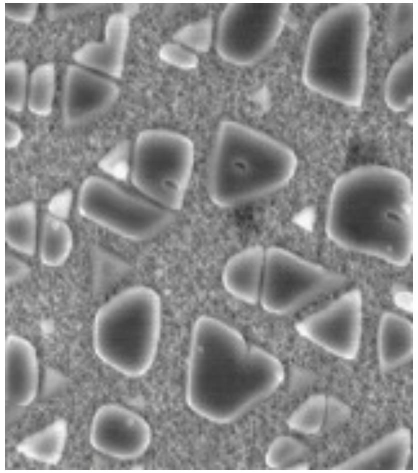
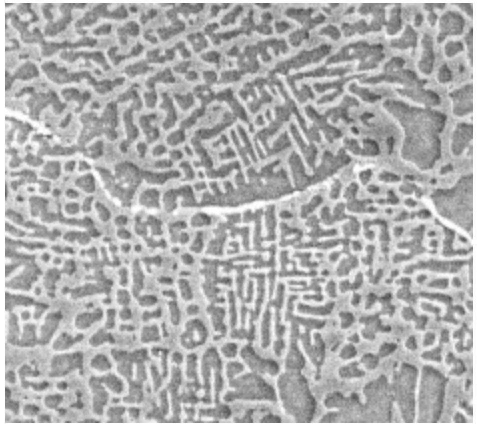
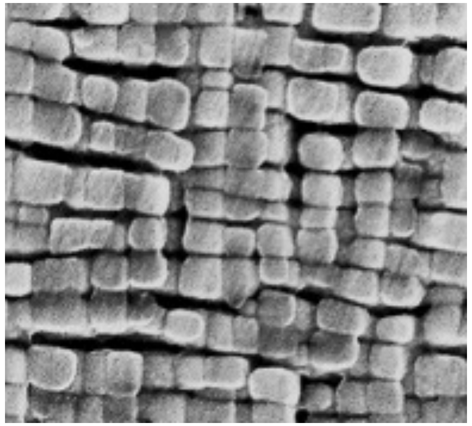
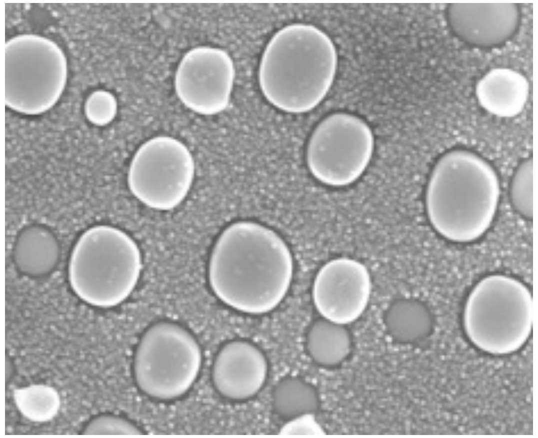
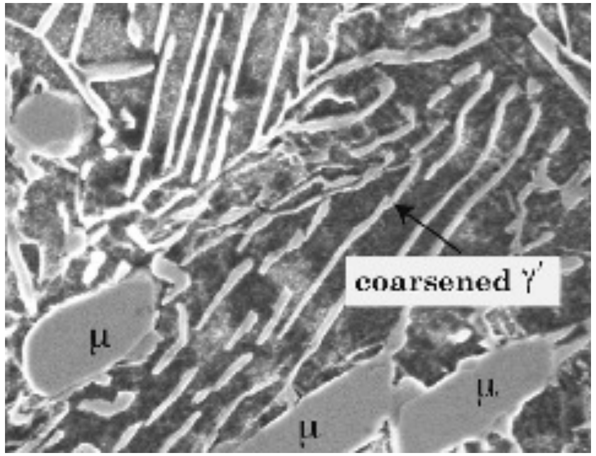
The digital microstructures are already binary images.

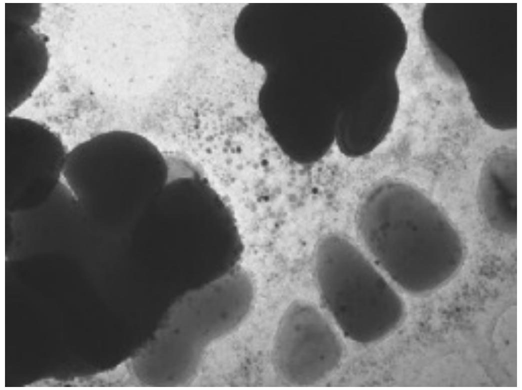
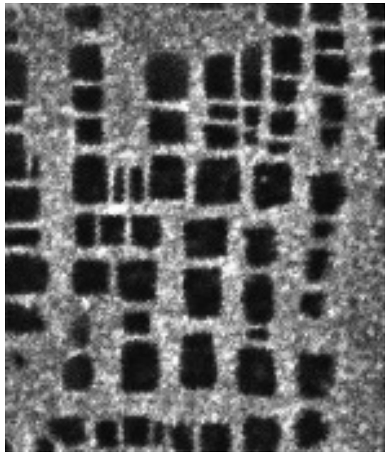
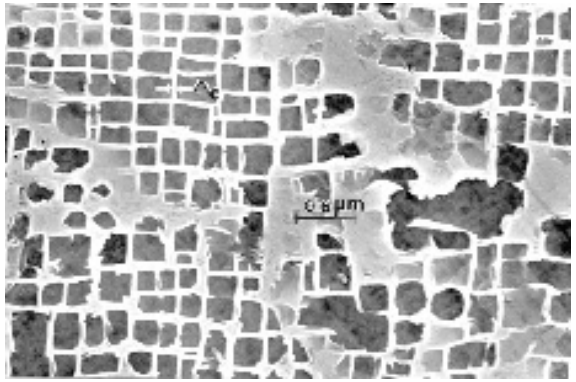
The experimental microstructures are greyscale images, which require additional steps for calculating two-point correlations.

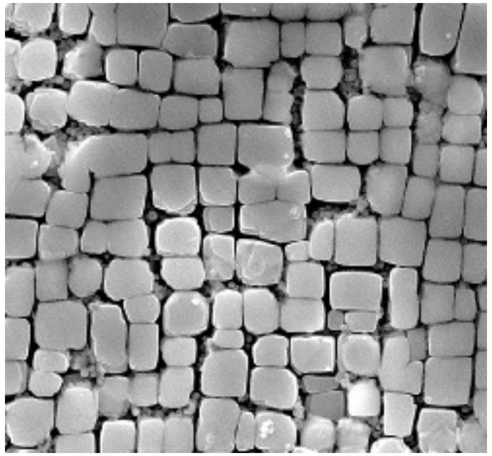


Khatavkar et al. 2020.

Case Study 2 – Hardness from experiments

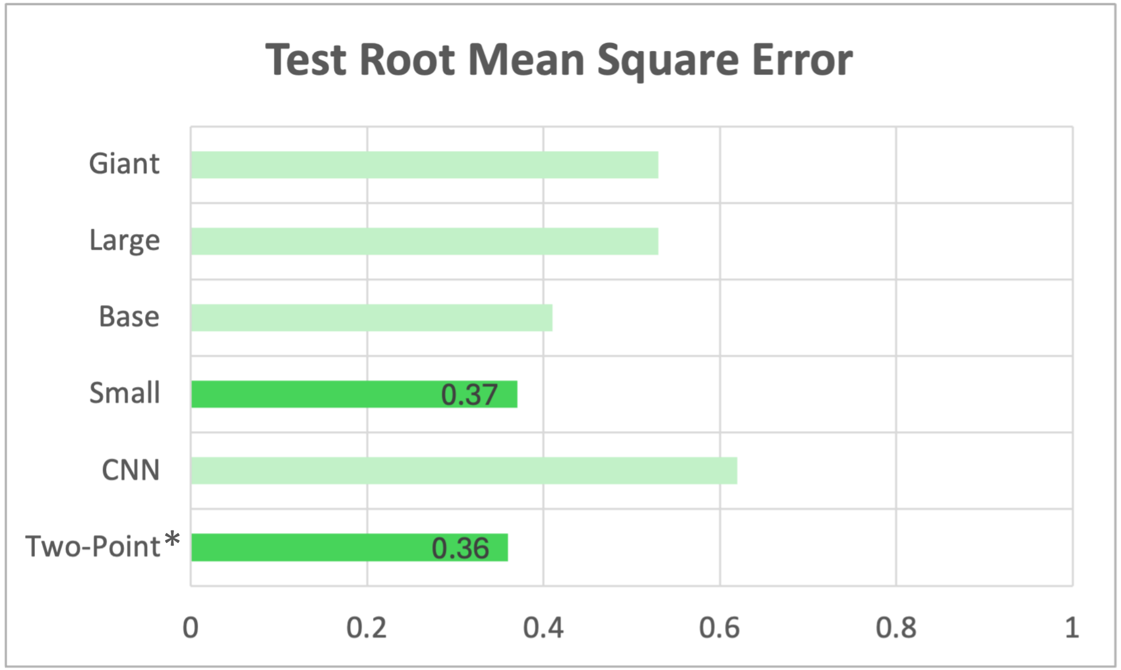


103 experimental microstructures and their corresponding Vickers Hardness values

Zhang et al. 2018. Bocchini et al. 2017. Yan et al. 2014. Mitchell et al. 2008. Zhong et al. 2013. Hongyu et al. 2010. Mignanelli et al. 2014. Huda 2009. Peng et al. 2018. Barbosa et al. 2005. Murr et al. 2013.

Case Study 2: Results

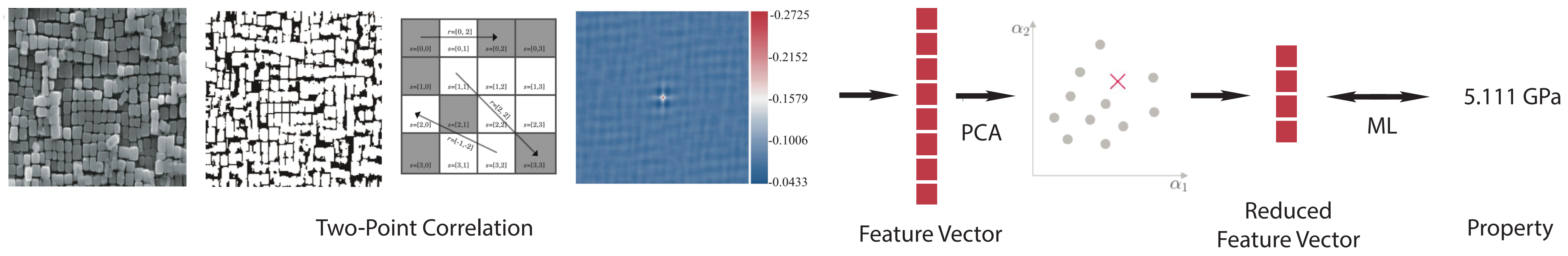
- The best DinoV2 model is the small model with 28 principal components.
- The two-point correlation function outperformed the best DinoV2 small model by 1%.

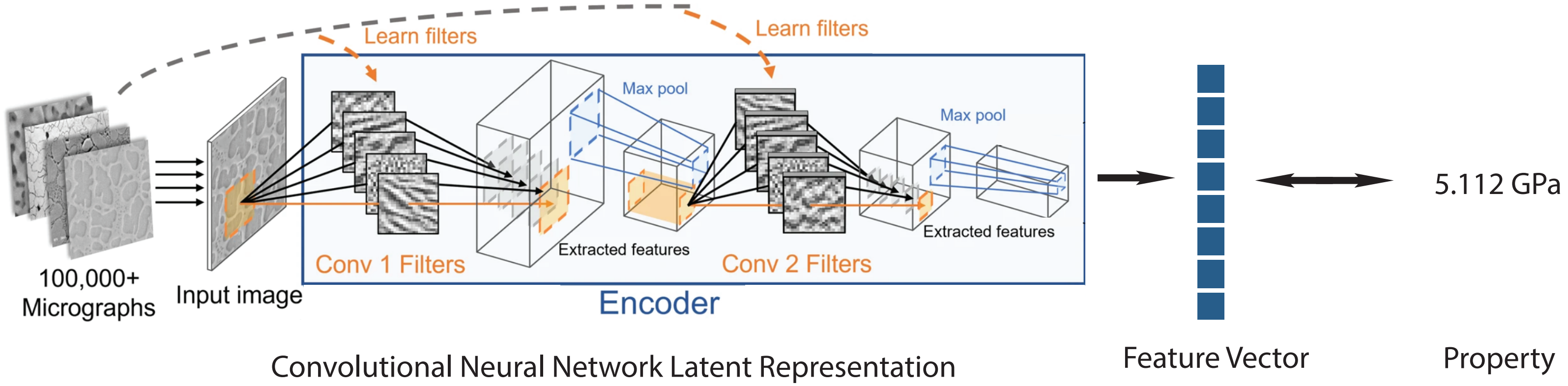


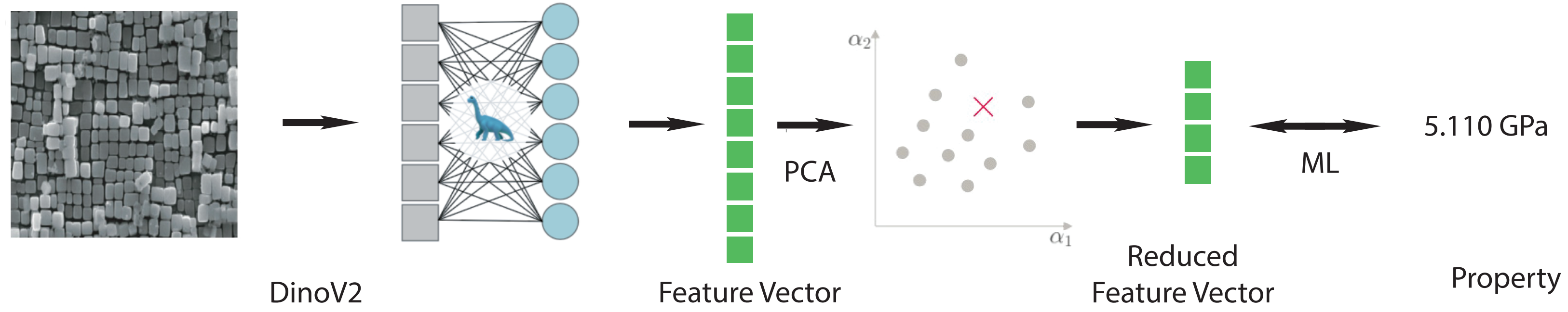
Parity plot showing the prediction results of the small DinoV2 model.

* As reported in Khatavkar et al. 2020.

Summary







Khatavkar et al. 2020. Stuckner et al. 2022.

Questions?

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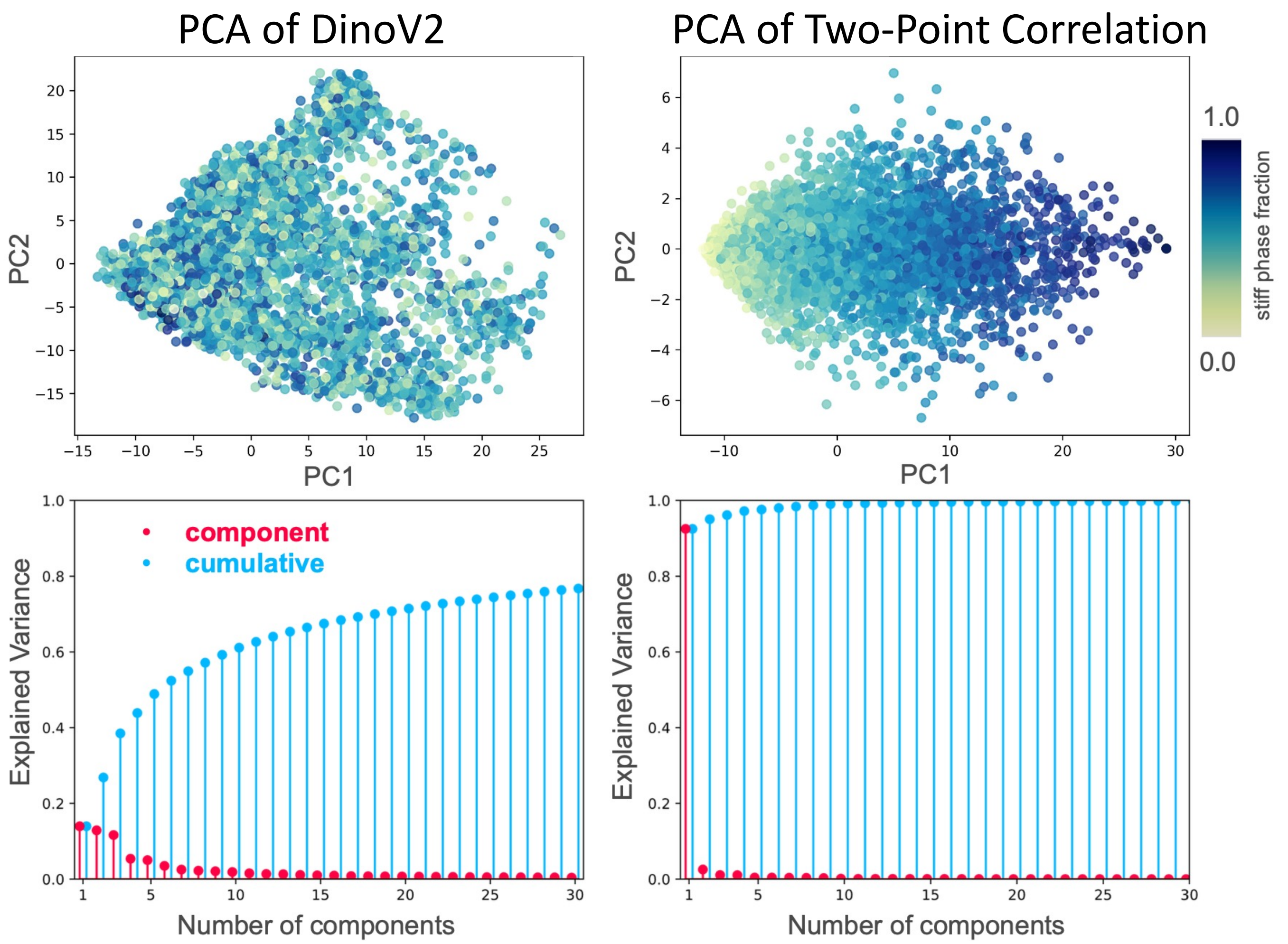
- Sheila Whitman: sheilaw@arizona.edu

Come say hi at the poster session #156!

Simulated Dataset – Feature Exploration

- The two-point correlation function prioritize the phase volume fraction
- The principal components of DinoV2 features are more balance in terms of explained variance.



Experimental Dataset - Feature Exploration

Analyzing the first two principal components provides insight into what DinoV2 features represent.