Explainable Machine Learning in Materials Mechanics

When the model itself becomes the source of knowledge instead of the data

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MecaNano COST Action CA21121

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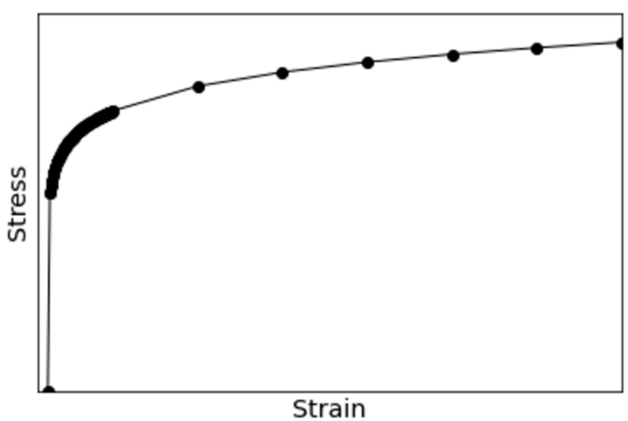
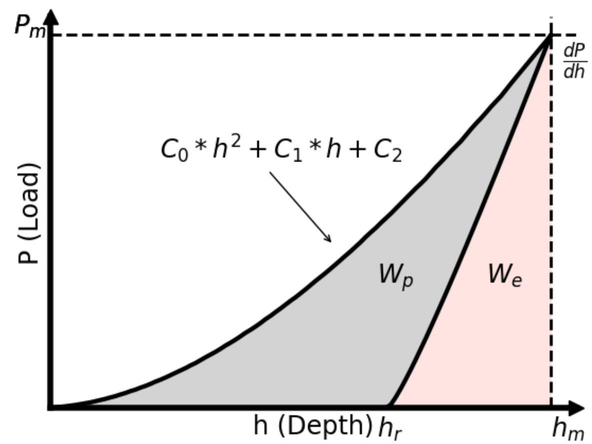
ESI

Examples

NANOINDENTATION THE ONE STOP SHOP FOR MATERIAL PROPERTIES?



Vs.

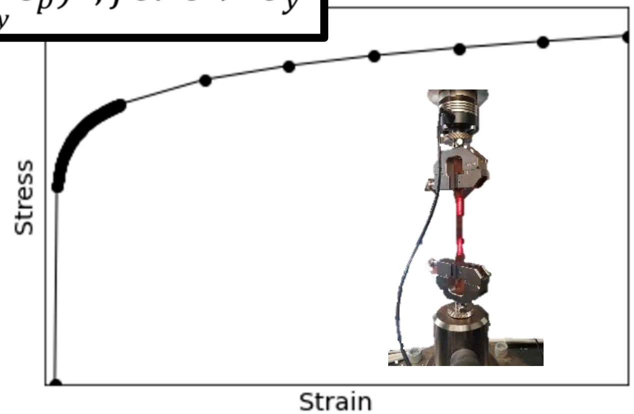


- Nearly non-destructive
- Rapid to perform
- No need for specialised sample geometry

Inverse-Problem

$$\sigma = E\varepsilon, for\ \sigma \leq \sigma_y$$

$$\sigma = \sigma_y\left(1 + \frac{E}{\sigma_y}\varepsilon_p\right)^n, for\ \sigma > \sigma_y$$



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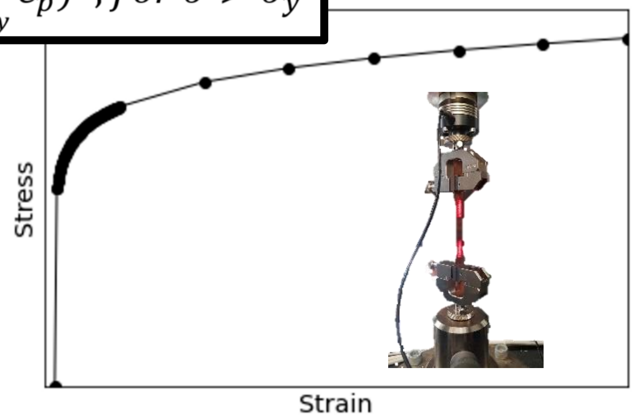
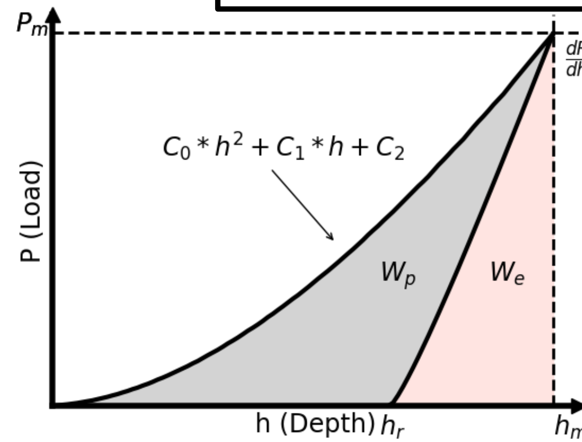


Elastic Modulus
Hardness



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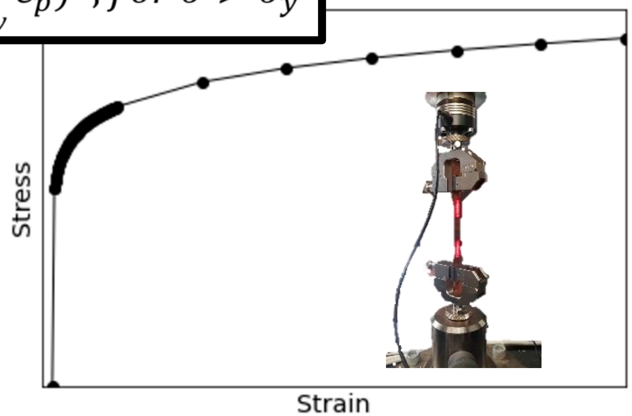

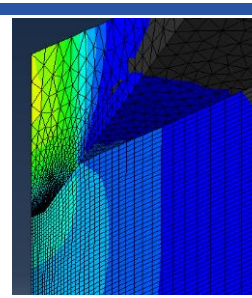

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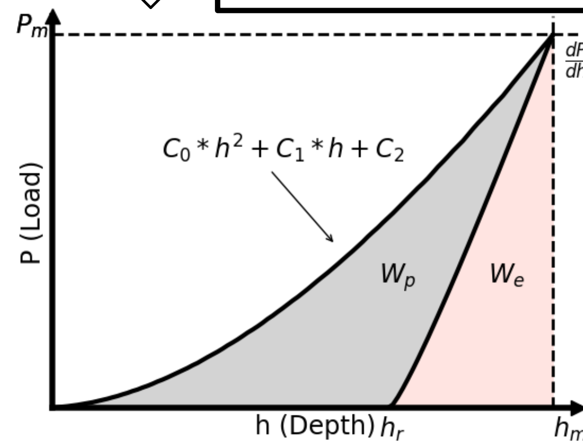

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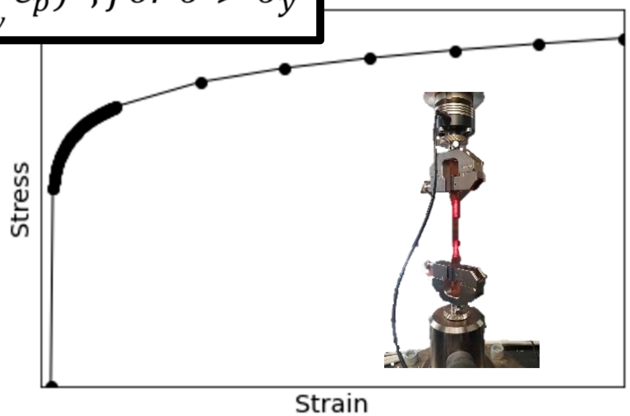

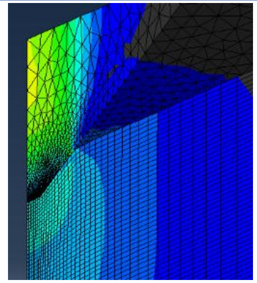

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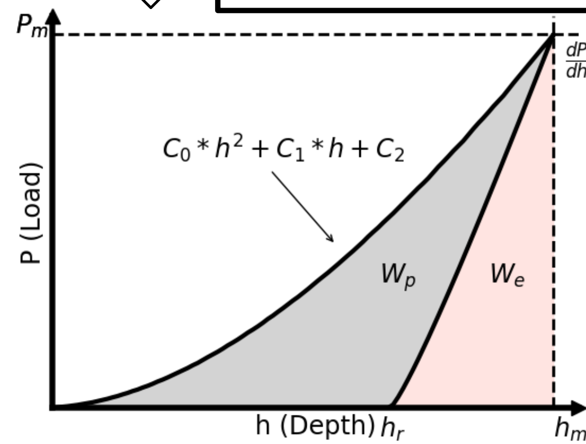

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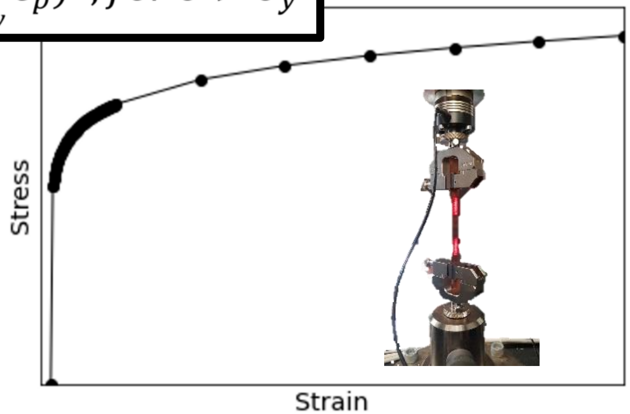

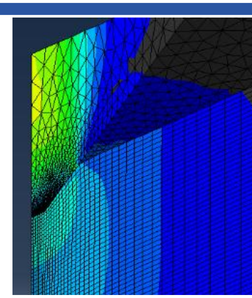

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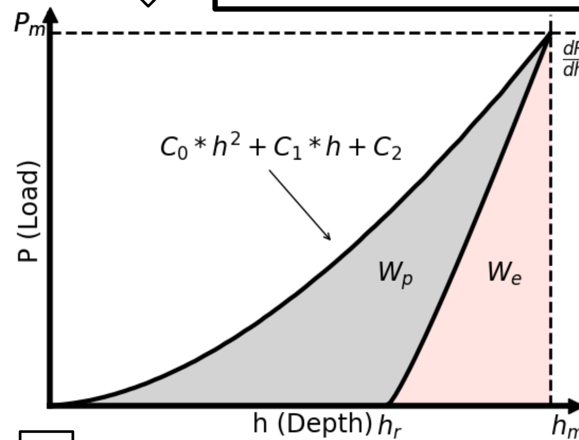

Methods

- Analytical Formulas
- Dimensional analysis (Π-Theorem)
- Optimisation algorithms
- Databases
- Machine Learning

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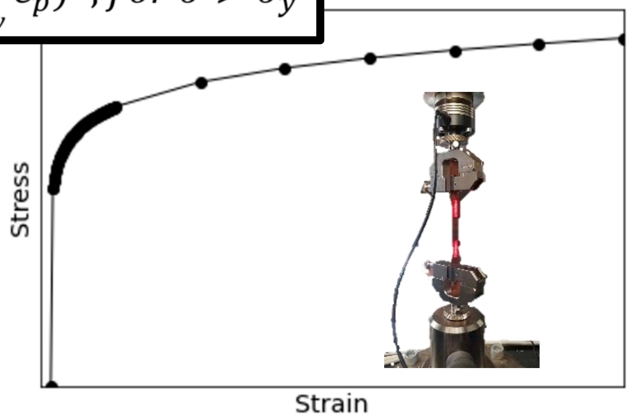

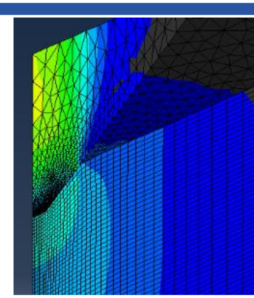

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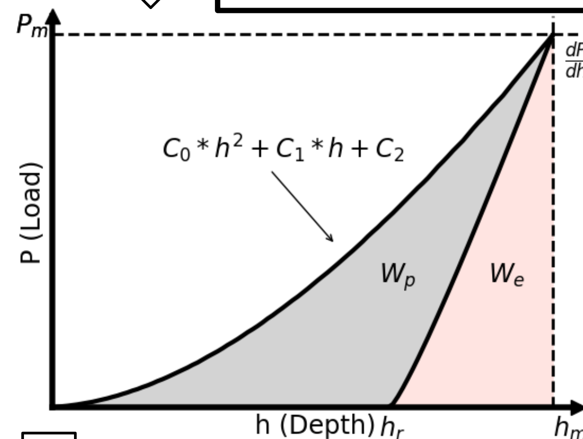

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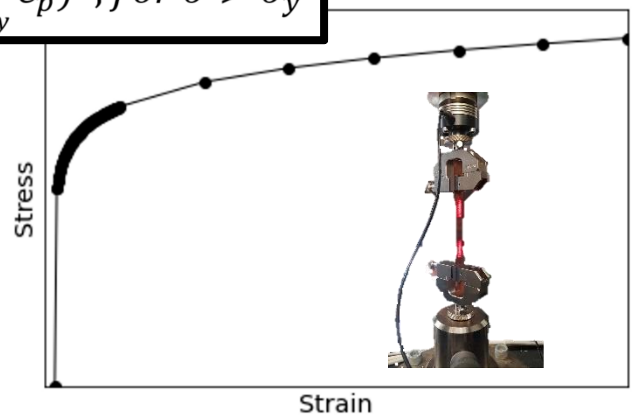

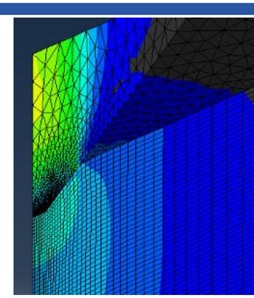

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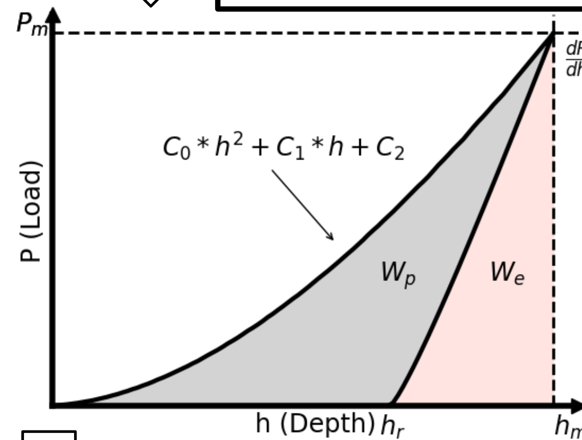

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1999 Huber and Tsakmakis

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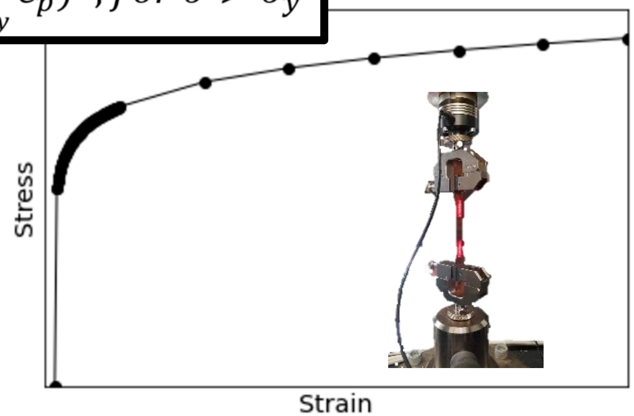
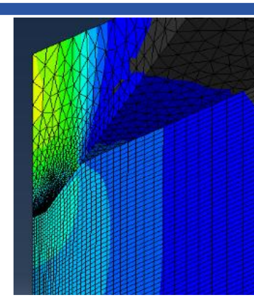
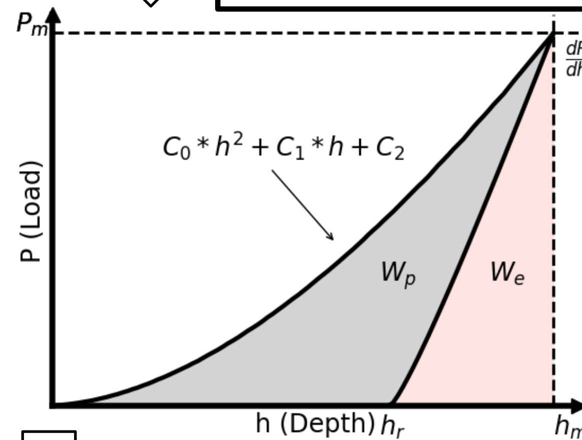




Tip Radius

Elastic Modulus
Hardness



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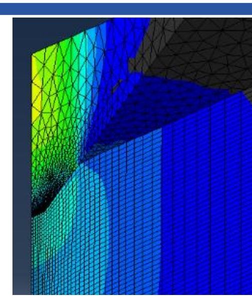

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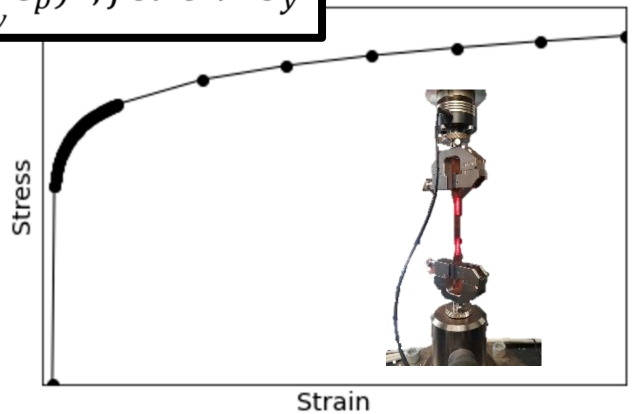

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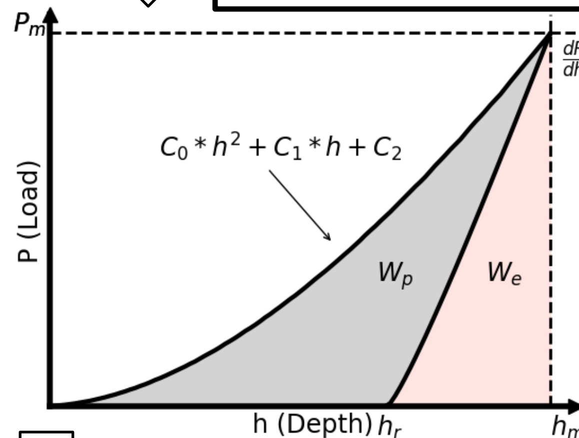

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Feature extraction:

- ✓ Unloading Slope
- ✓ Loading Curvature
- ✓ Plastic & Elastic Work
- ✓ Work Ratio
- ✓ Normalized Features

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Dimensional Analysis

- Construction of dimensionless universal functions by identifying base quantities & units.

$$P = P(h, E, \nu, E_i, \nu_i, \sigma_y, n)$$

e.g. fluid mechanics
Reynolds number

M. Dao, N. Chollacoop, K. J. van Vliet, T. A. Venkatesh, and S. Suresh, "Computational modeling of the forward and reverse problems in instrumented sharp indentation," Acta Materialia, vol. 49, no. 19, pp. 3899–3918, 2001, doi: 10.1016/S1359-6454(01)00295-6
Fridrich Kick, Kick, Das Gesetz der proportionalen Widerstände und seine Anwendungen, nebst Versuchen über das Verhalten verschiedener Materialien bei gleichen Formänderungen sowohl unter der Presse als dem Schlagwerk. Leipzig: Art. Felix, 1885.

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Kicks Law (1885)

$$\boxed{C = \frac{P}{h^2}}$$

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$$\boxed{C = \frac{P}{h^2}} = \sigma_r \Pi\left(\frac{E^*}{\sigma_r}, n\right)$$

C ... deflection of loading curve,

σ_r … representative stress

Π ()… dimensionless function

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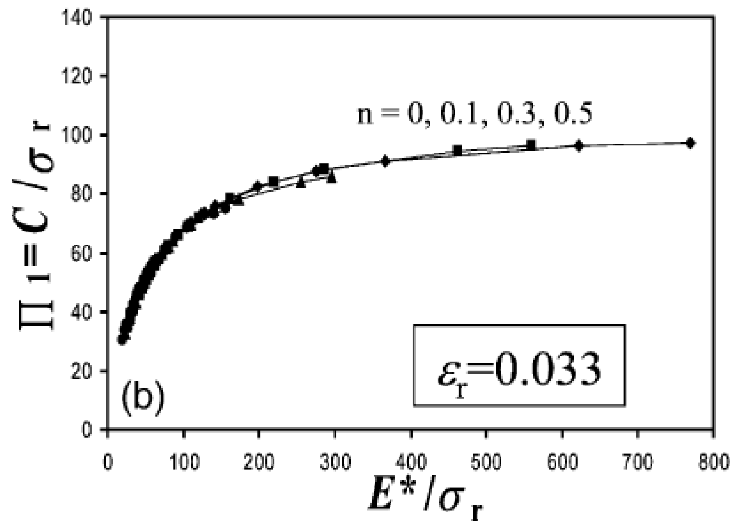

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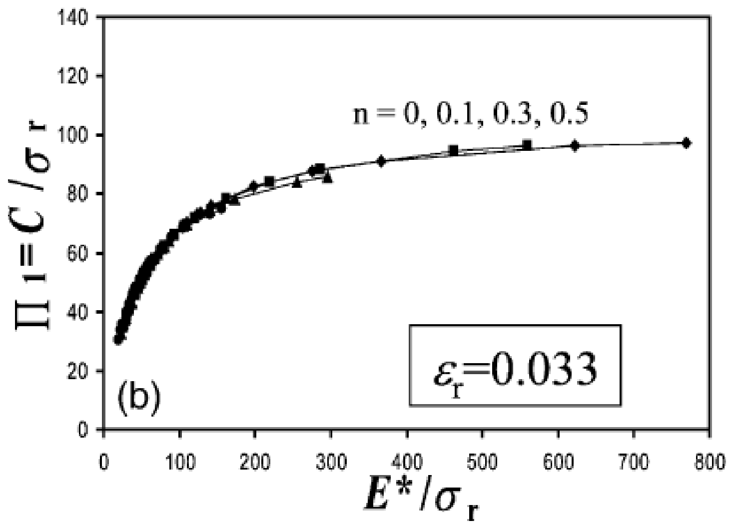

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Calibrated by FEM, number of experiments is unfeasible!

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Problems with the inverse problem

- Mystical Materials

True Mystical:
Different Input
Parameters

Meng, L., Breitkopf, P., Raghavan, B. *et al.* On the study of mystical materials identified by indentation on power law and Voce hardening solids. *Int J Mater Form* **12**, 587–602 (2019). https://doi.org/10.1007/s12289-018-1436-1
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Problems with the inverse problem

- Mystical Materials

True Mystical:
Different Input
Parameters

False Mystical:
Similar Input
Parameters

Different parameter combinations can lead to the same Indentation Curve!

Not only a Mathematical but also a Materials Scientific Problem!

Lack of trust in BLACK BOX models.

Meng, L., Breitkopf, P., Raghavan, B. *et al.* On the study of mystical materials identified by indentation on power law and Voce hardening solids. *Int J Mater Form* **12**, 587–602 (2019). https://doi.org/10.1007/s12289-018-1436-1
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CLASSIFICATION OF NANOINDENTATION DATA OF MULTIPHASE MATERIALS

Claus O. W. Trost[1,2]

Stanislav Žák[1]

Lukas Walch[4]

Sebastian Schaffer[2,3]

Lukas Exl[2,3]

Megan J. Cordill[1]

[1]Erich Schmid Institute, Austrian Academy of Sciences, Leoben, Austria

[2]Cross Disciplinary Platform for Machine Learning, Austrian Academy of Sciences, Vienna, Austria

[2]Wolfgang Pauli Institute, Faculty of Mathematics, University of Vienna, Austria.

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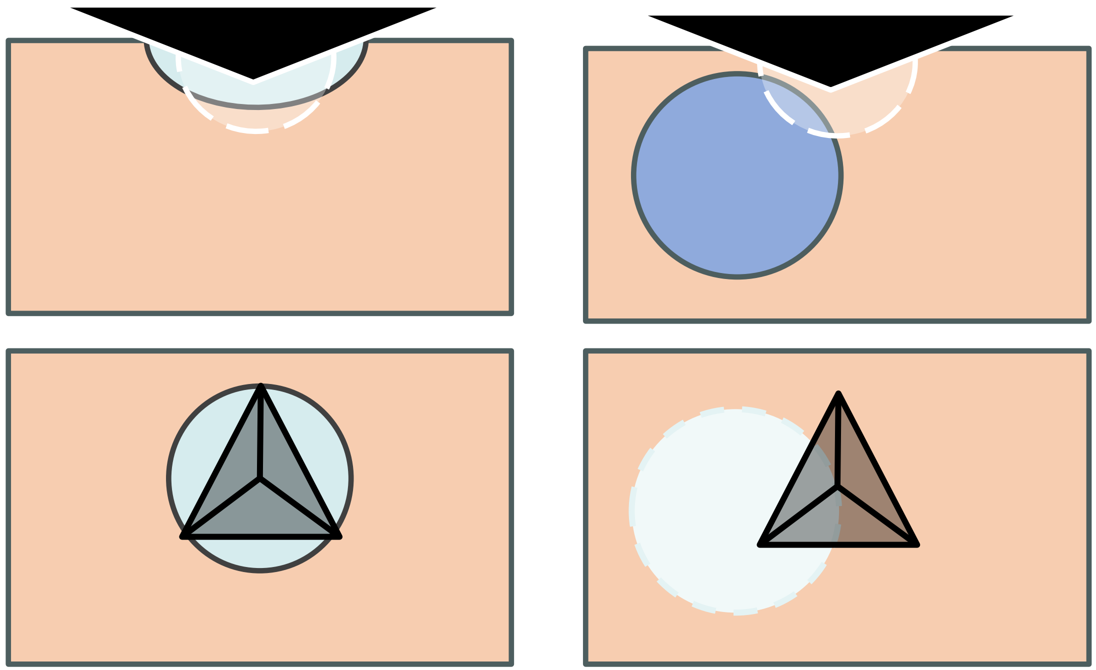
CLASSIFICATION OF NANOINDENTATION DATA OF MULTIPHASE MATERIALS

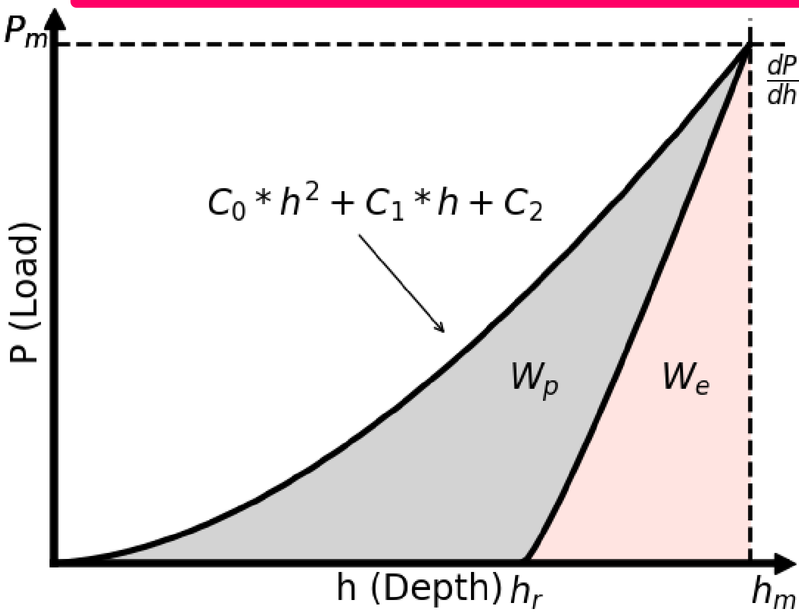
Influence in the measurements

- Surroundings
- Sub-surface features



What can we learn from the classification of indentation data?

Are the usually chosen features good enough?

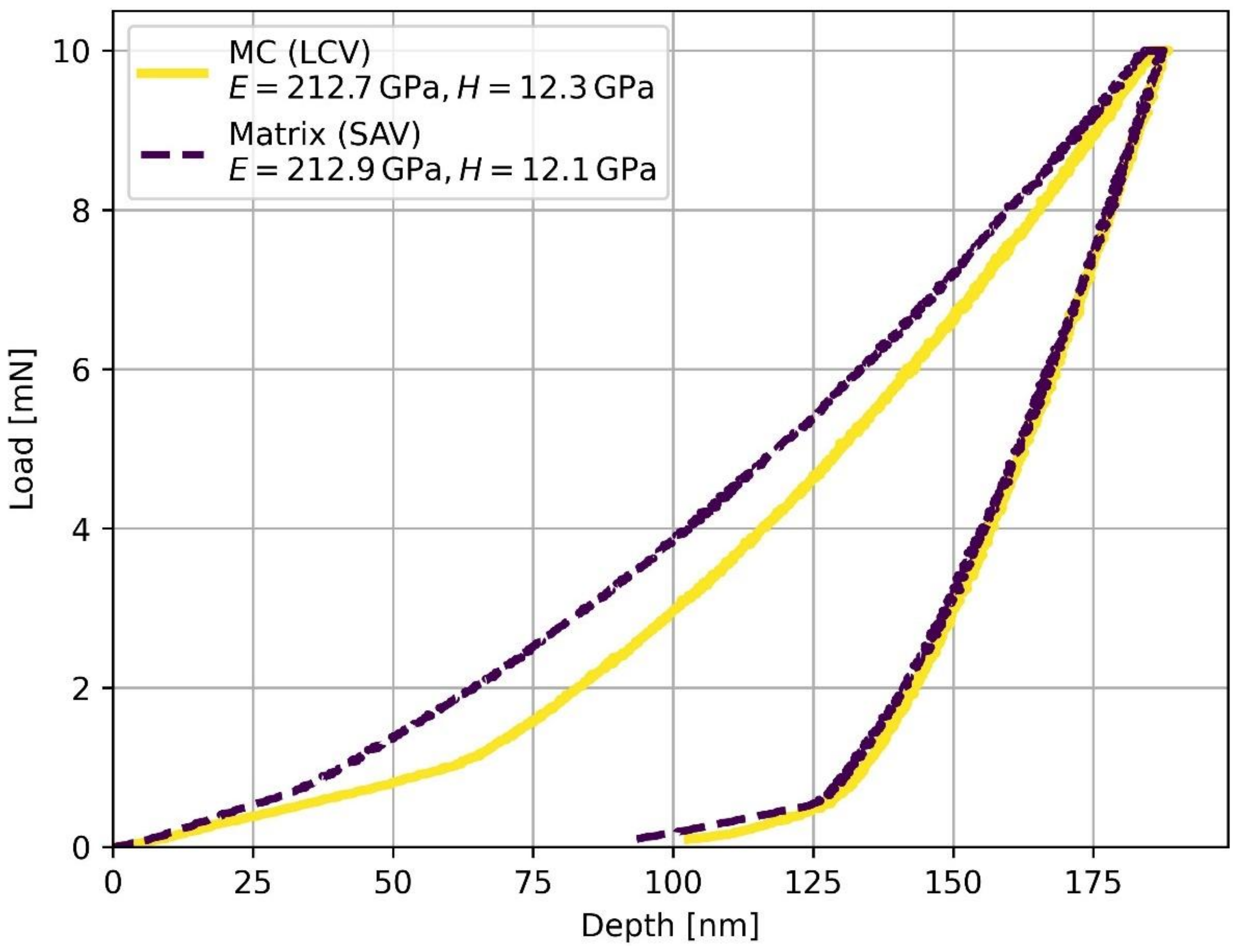


$$E_r = \frac{dP}{dh}\frac{\sqrt{\pi}}{2\beta\sqrt{A}}\sqrt{\frac{A_\mathrm{i}}{A}}$$

$$H = \frac{P}{A}\left(\frac{A_\mathrm{i}}{A}\right)$$

Why the complete curve?

How would you distinguish these indents?



Investigated Materials

voestalpine
ONE STEP AHEAD.

BÖHLER S390 MICROCLEAN

Fe	C	W	Mo	V	Co	Cr	Si	Mn	wt.%
68.5	1.6	10.4	2.0	4.8	8.0	4.8	0.6	0.3	

66 HRC

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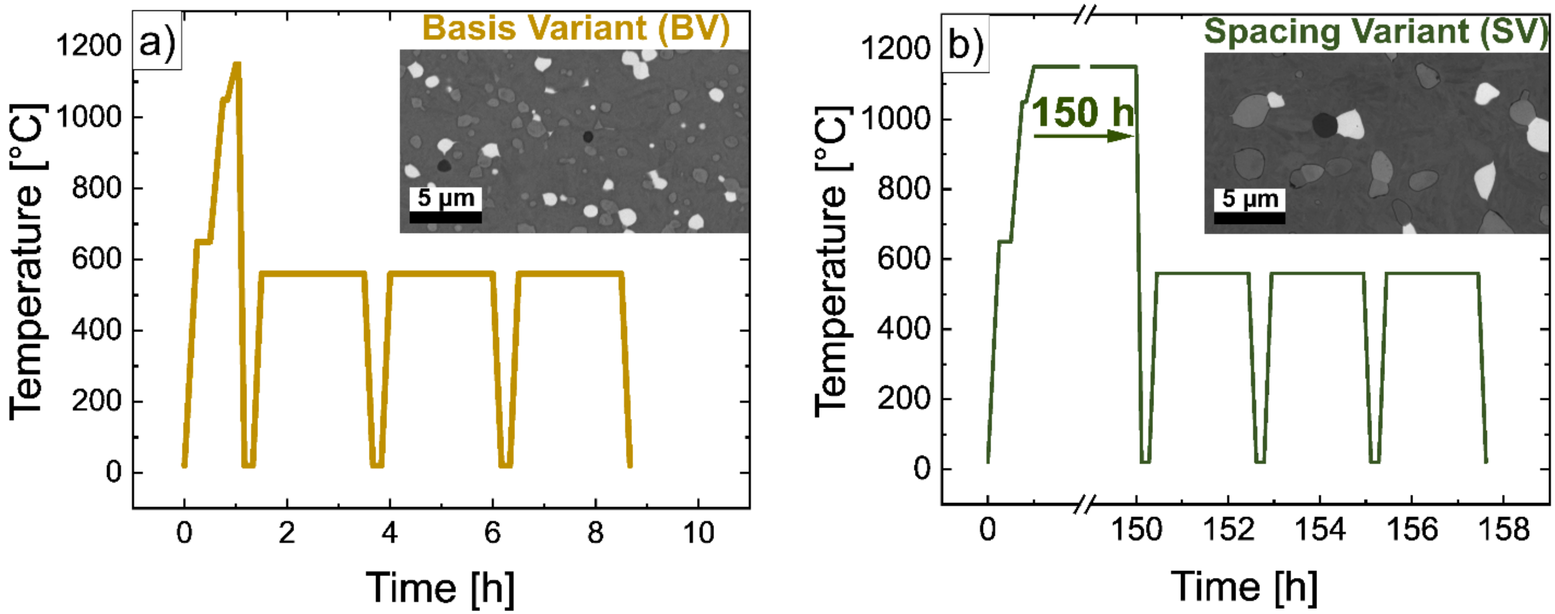
Investigated Materials

voestalpine
ONE STEP AHEAD.

- Basis Variant (BV)
- Spacing Variant (SV),
- Low Carbide Variant (LCV)
- Retained Austenite Variant (RAV)

BÖHLER S390 MICROCLEAN



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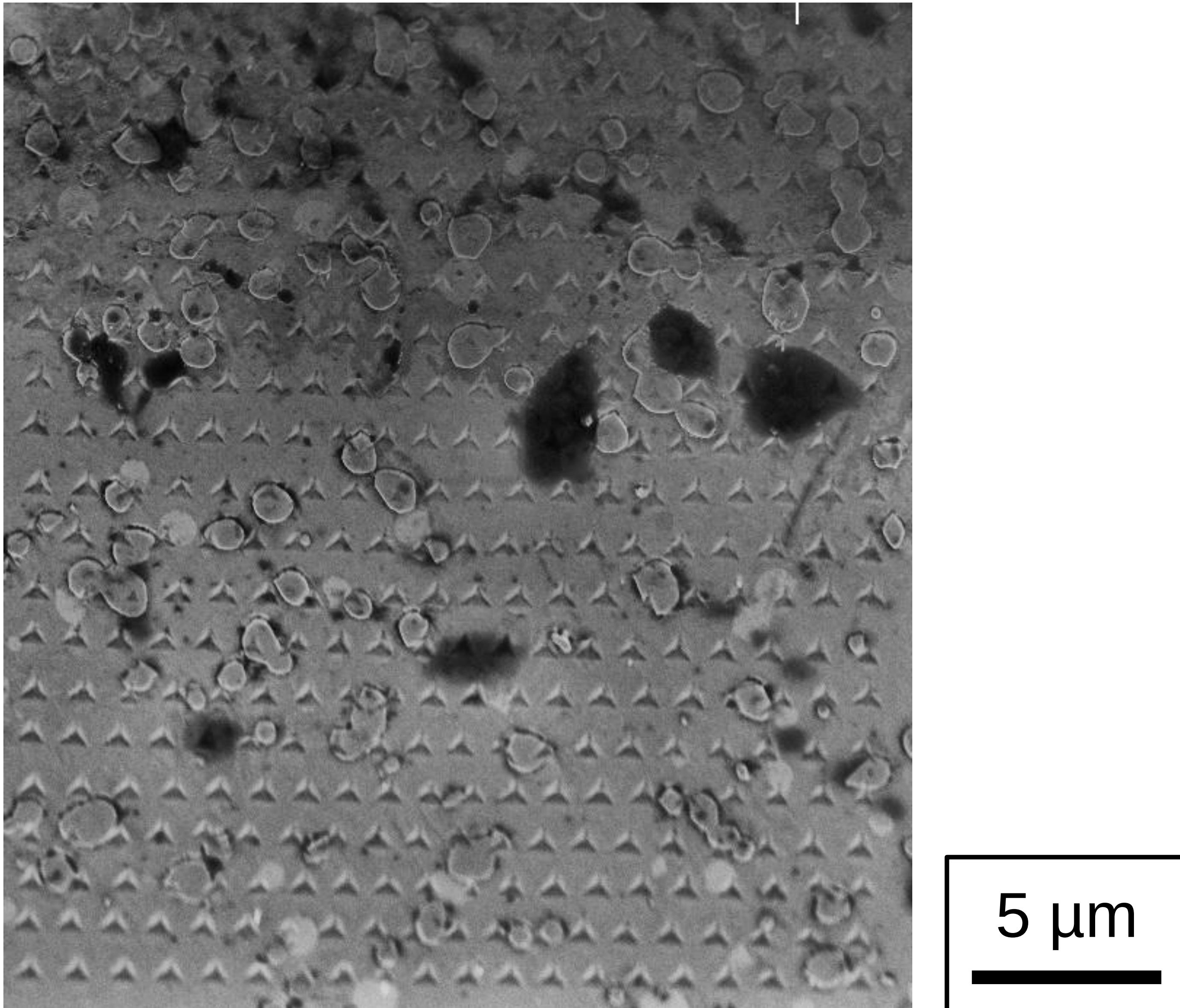
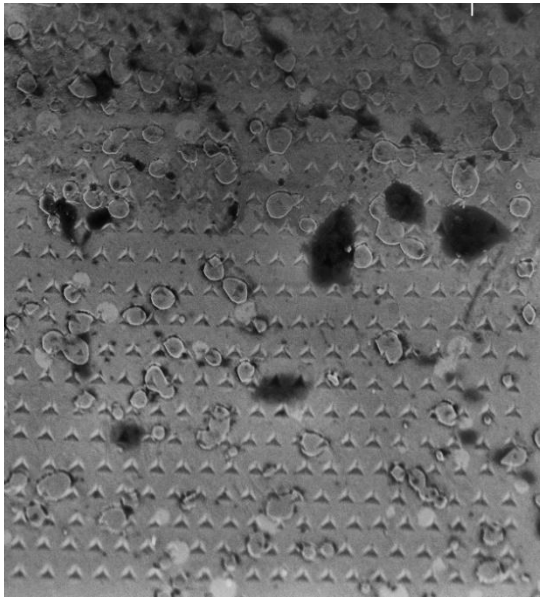
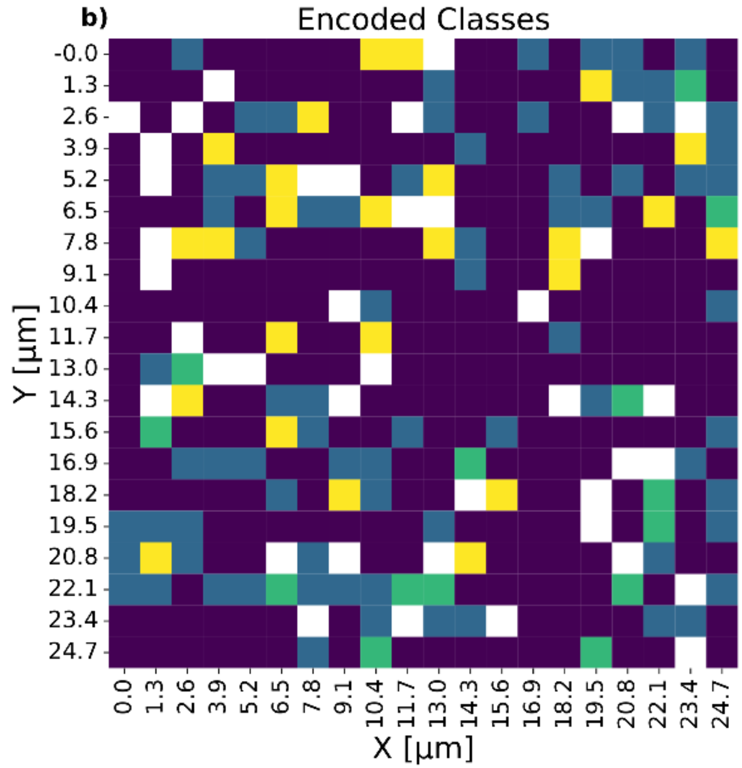
Indenting Multiphase Materials



Disentangling Properties of Multiphase Materials



Labelling



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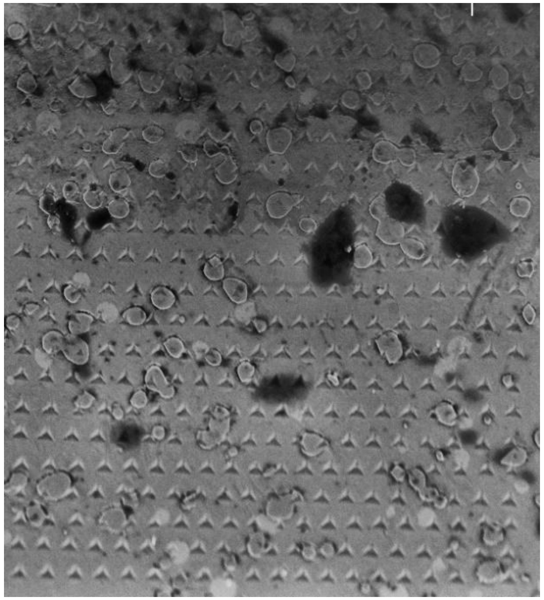
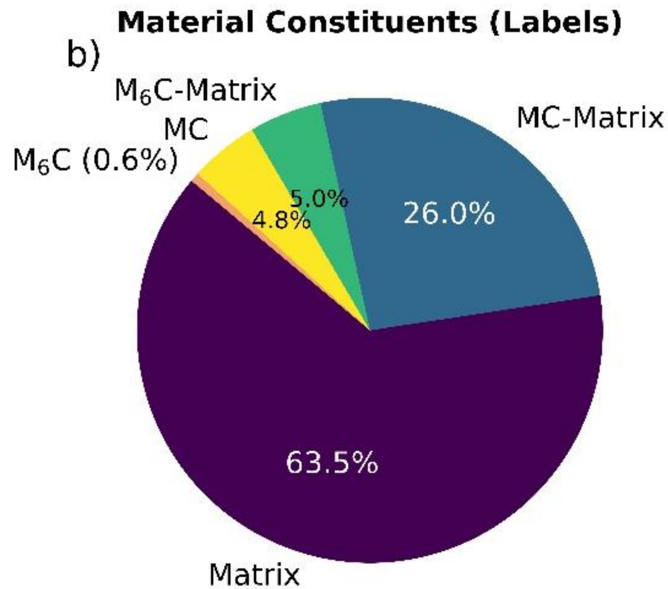
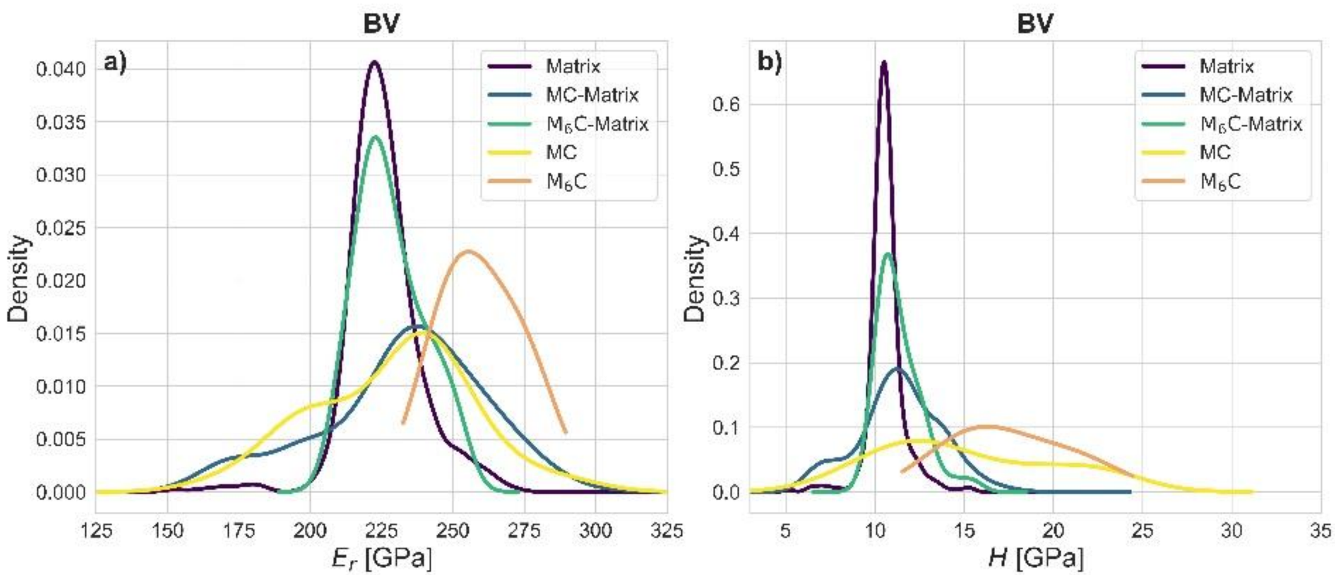
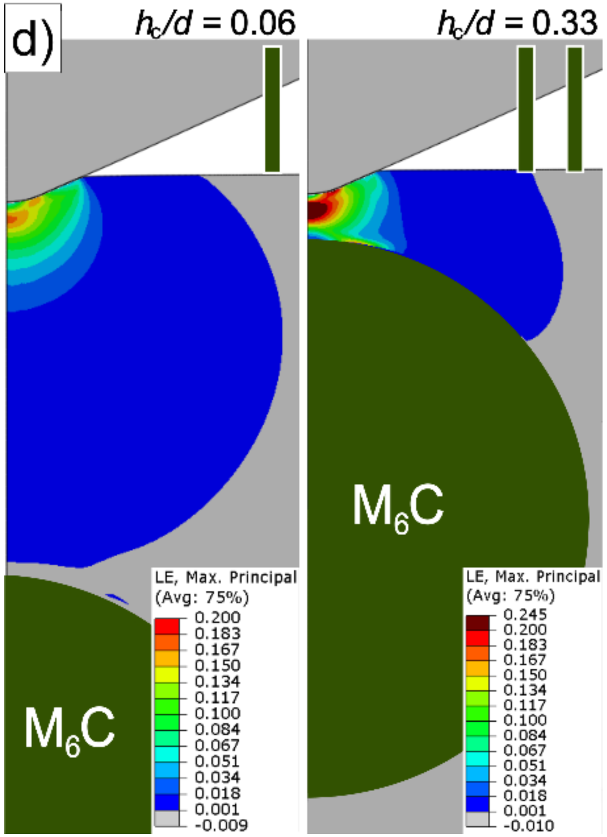


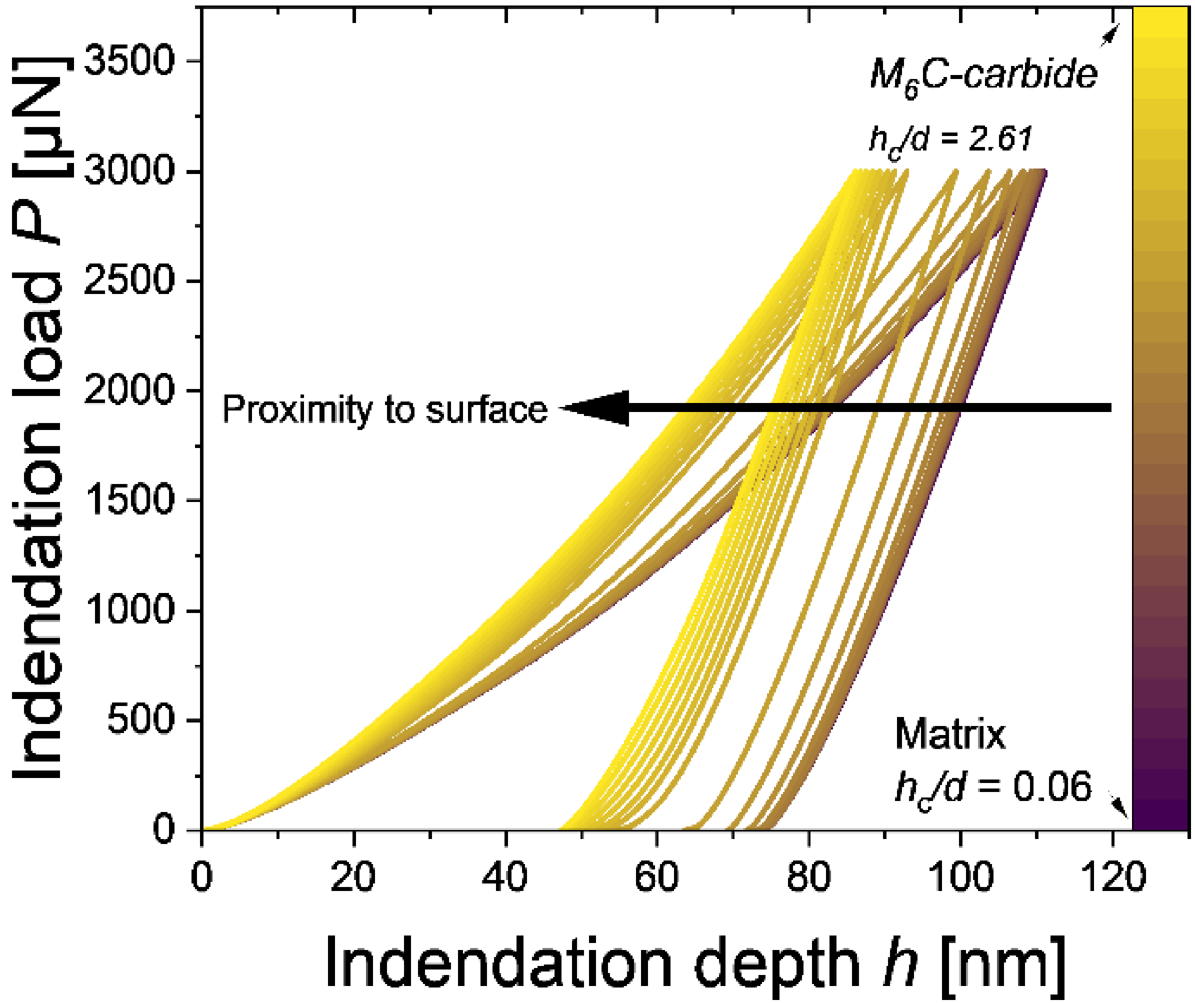




Kernel Density Estimation

Why Mixed Classes?

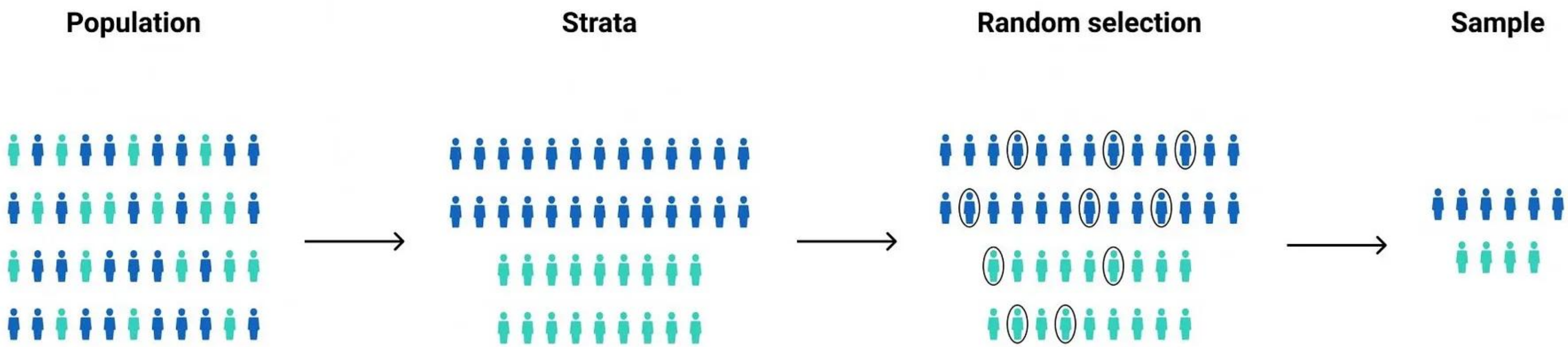


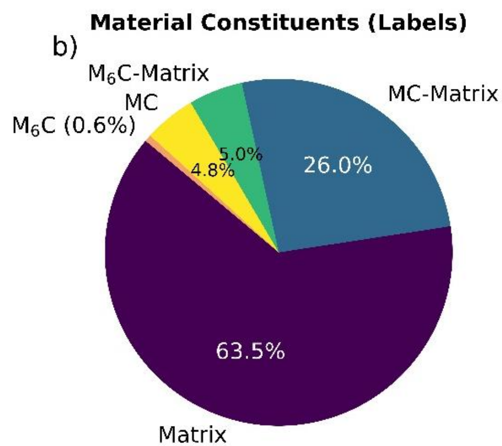


L. Walch, C. O.W. Trost, K. Kutlesa, J. Zitz, T. Klünsner, G. Ressel, A.Hackl, M. J. Cordill, S. Zak; ***"Sensing Particles Under the Surface with Nanoindentation"***, under Review, Materials and Design, 2025

Model Selection & Hyperparameter Tuning

- Randomized Search Cross Validation
- Including Stratification



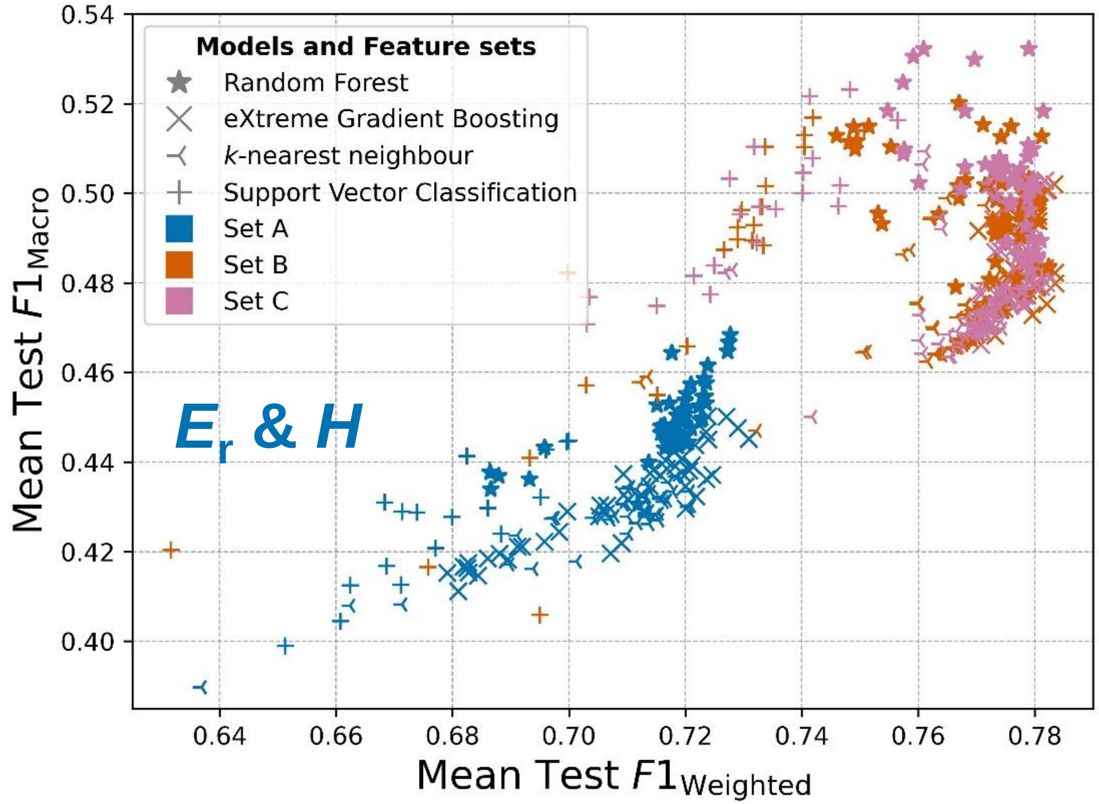


https://medium.com/analytics-vidhya/stratified-sampling-in-machine-learning-f5112b5b9cfe

Model Selection, Hyperparameter Tuning and Feature Selection

- Randomized Search Cross Validation
- Including Stratification

$$F_1 = 2\frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} = \frac{2\text{TP}}{2\text{TP} + \text{FP} + \text{FN}}.$$



Dimensional Analysis and E_r & H

Model Selection, Hyperparameter Tuning and Feature Selection

- Randomized Search Cross Validation
- Including Stratification

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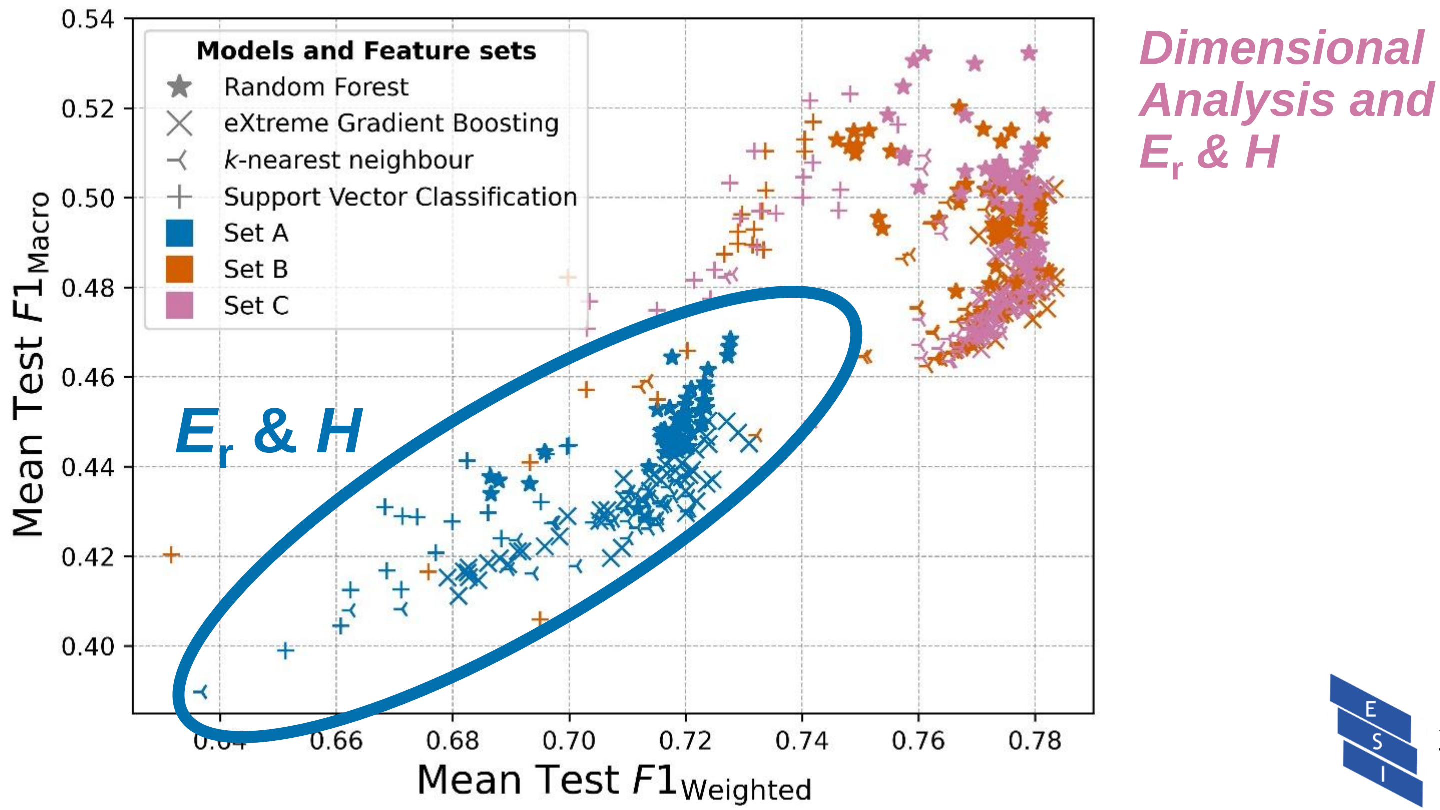
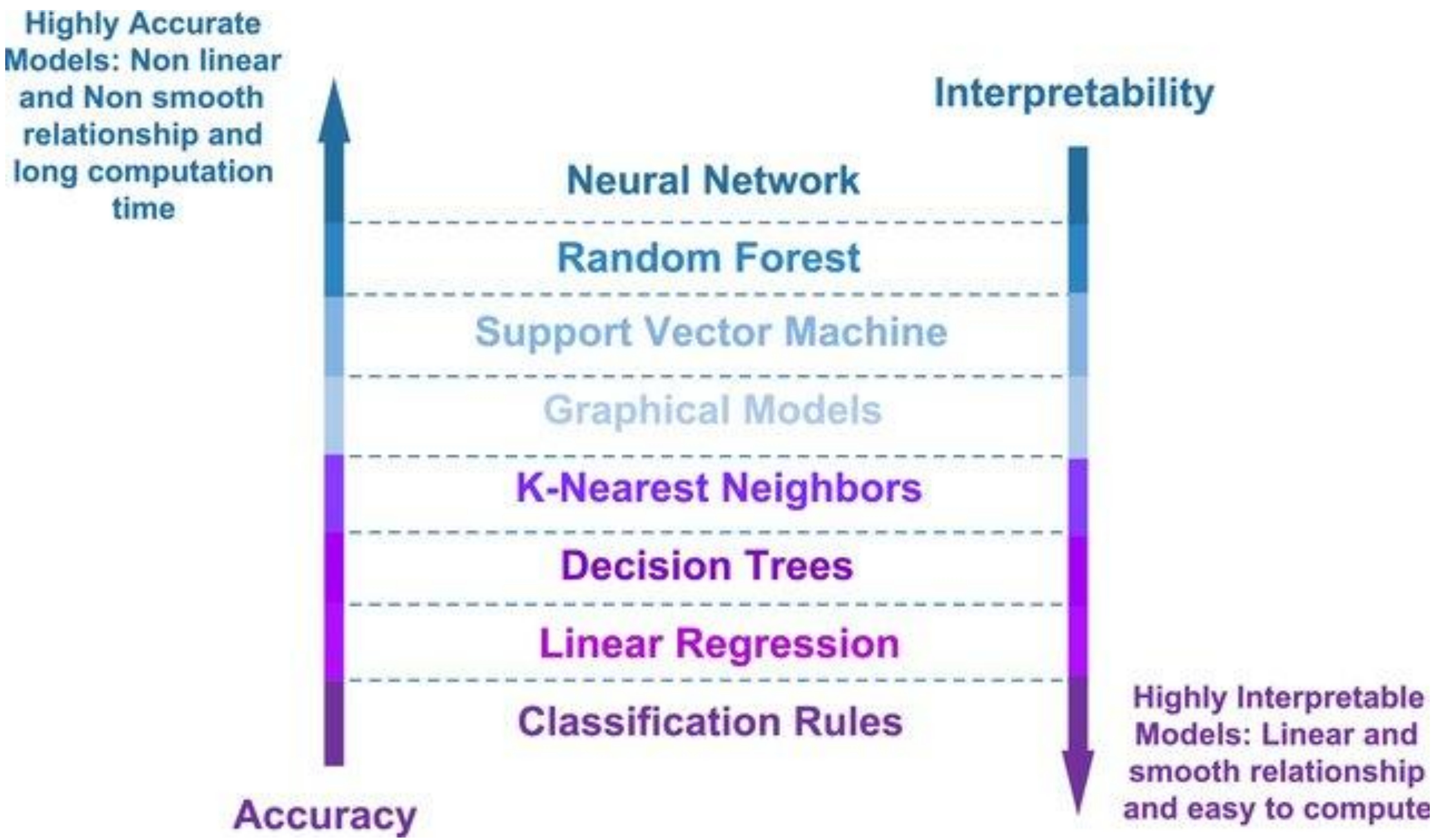


Interpretability vs. Accuracy



Fourati, H., Maaloul, R. & Chaari, L. **A survey of 5G network systems: challenges and machine learning approaches**. *Int. J. Mach. Learn. & Cyber.* **12**, 385–431 (2021). https://doi.org/10.1007/s13042-020-01178-4

SHAP (SHapley Additive exPlanations)

- Based on Shapley values from **cooperative game theory.**

- Used in data science to e.g. by banks when explaining basis of loan rejection to customer or in medical field to assist during operations

Enables <u>model agnostic</u> interpretation of complex models

[5] S. Lundberg and S.-I. Lee, "A Unified Approach to Interpreting Model Predictions," 2017. [Online]. Available: https://arxiv.org/pdf/1705.07874
[6] https://towardsdatascience.com/one-feature-attribution-method-to-supposedly-rule-them-all-shapley-values-f3e04534983d

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About 49,000 citations since 2017

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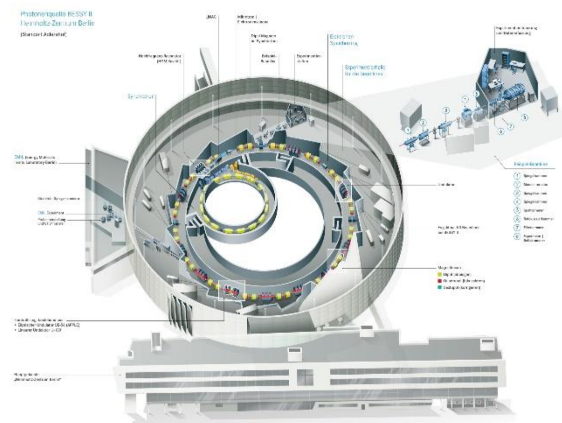
[6] https://towardsdatascience.com/one-feature-attribution-method-to-supposedly-rule-them-all-shapley-values-f3e04534983d
[7] https://www.mcicon.com/

Shapley Values



Work together in different sets at Beam time.

- Different experimental experience
- Different amount of samples in different combinations
- Every sample pays same amount of money → 5€

Fair way to split money per sample if we work together?

https://www.helmholtz-berlin.de/forschung/quellen/bessy/wie-funktioniert-bessy_de.html

Shapley Values

Possible Sets	{}							
Number of Samples per hour	0	2	4	5	7	8	11	12

[8] Selçuk Özyurt, *(AGT4E10) [Game Theory] Shapley Value; York University, Department of Economics.* [Online]. Available: https://www.youtube.com/watch?v=HWRHKs3O_Us (accessed: Sep. 7 2022).

Shapley Values

Possible Sets	{}							
Number of Samples per hour	0	2	4	5	7	8	11	12

$$G = (N, v)$$

$$\emptyset_i(N, v) = \frac{1}{n!} \sum_{S \subseteq N\{i\}} |S|!\,(n - 1 - |S|)!\, \underbrace{[v(S \cup \{i\}) - v(S)]}_{\textit{marginal contribution of player i to coalition S}}$$

$|S|$ ... *# of elements in set S*

v ... *worth function*

N ... *set of players*

n ... *number of players*

$v(S \cup \{i\})$ ... *worth of coalition with player*

$v(S)$ ... *worth without player*

S ... *every coalition without player i*

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S ... *every coalition without player* i

The Shapley value of Claus is: 2
The Shapley value of Patrice is: 4.5
The Shapley value of Megan is: 5.5

[8] Selçuk Özyurt, *(AGT4E10) [Game Theory] Shapley Value; York University, Department of Economics.* [Online]. Available: https://www.youtube.com/watch?v=HWRHKs3O_Us (accessed: Sep. 7 2022).

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$N \ldots set\ of\ players$

$n\ \ \ldots number\ of\ players$

$v(S \cup \{i\}) \ldots worth\ of\ coalition\ with\ player$

$v(S) \ldots worth\ without\ player$

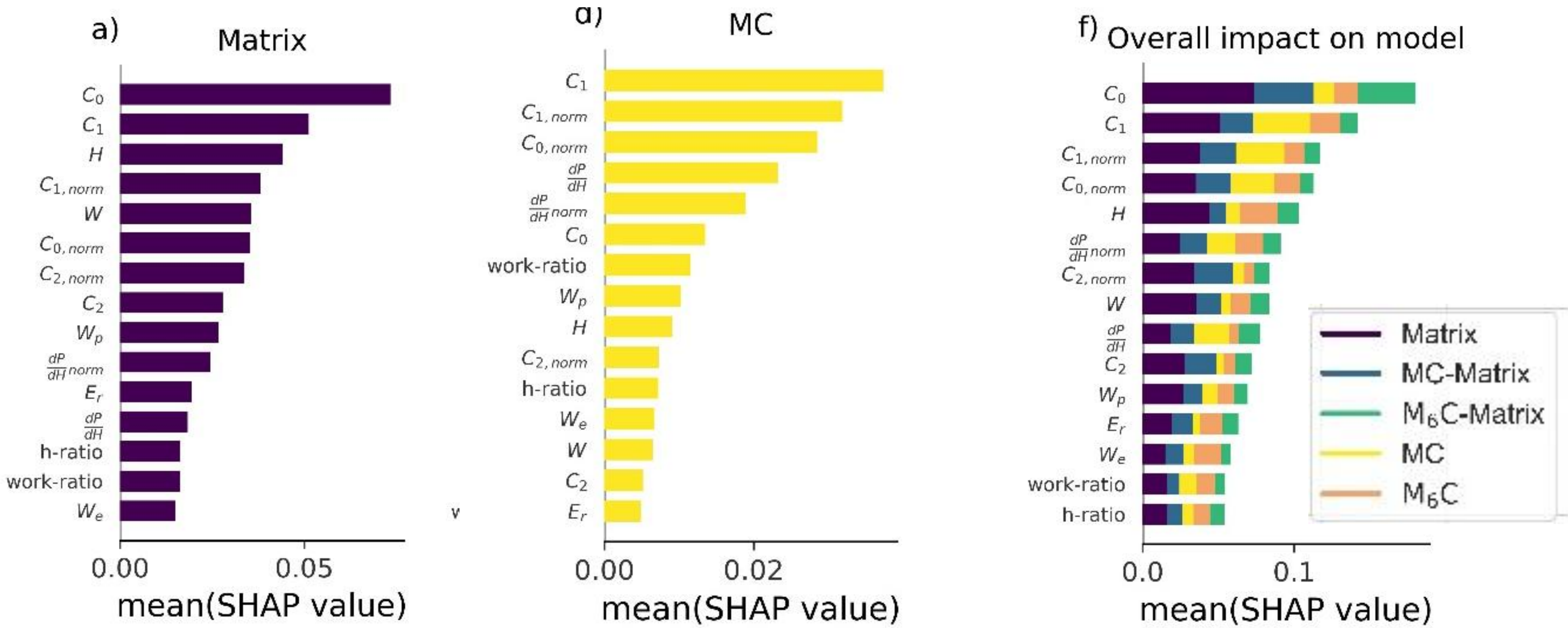
$S \ldots every\ coalition\ without\ player\ i$

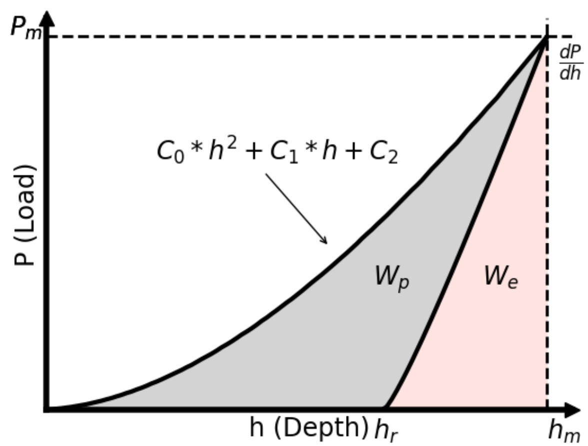
The Shapley value of Claus is: 2 → 10 €
The Shapley value of Patrice is: 4.5 → 22.5€
The Shapley value of Megan is: 5.5 → 27.5 €

Might be fair based on game theory but not in terms of labour laws!

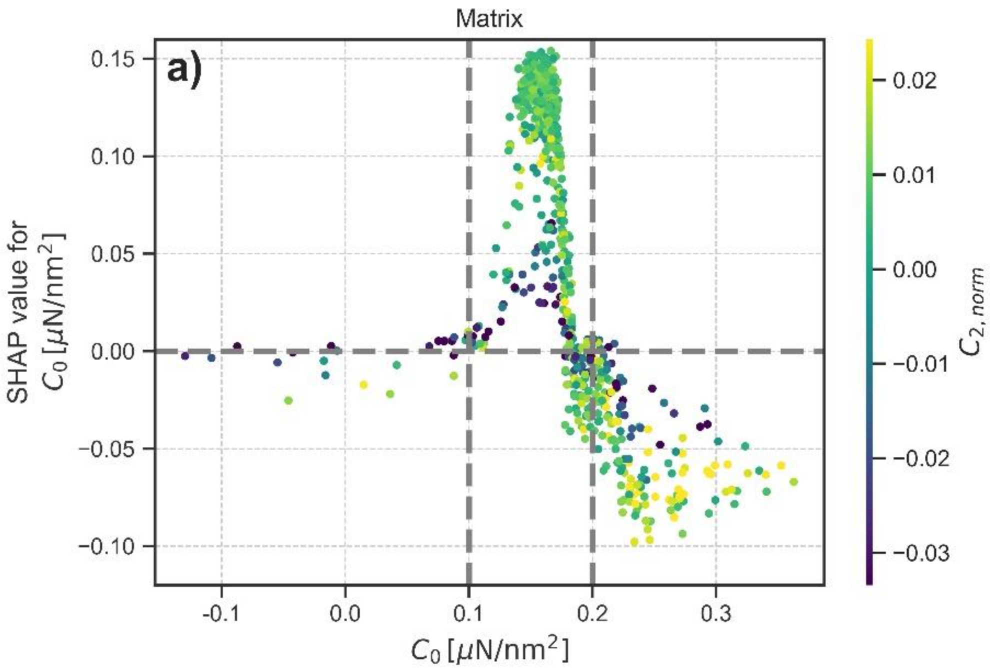
ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

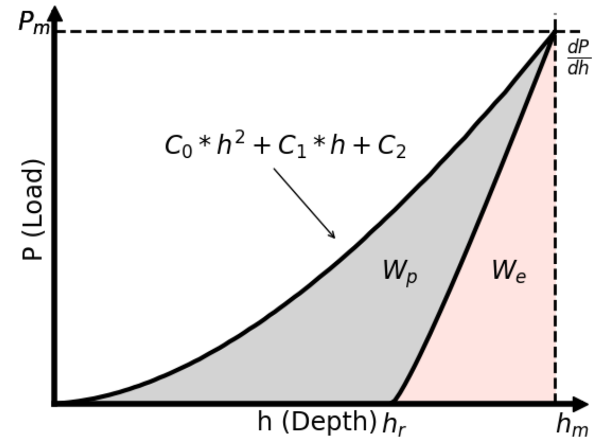
What can we learn from classification?



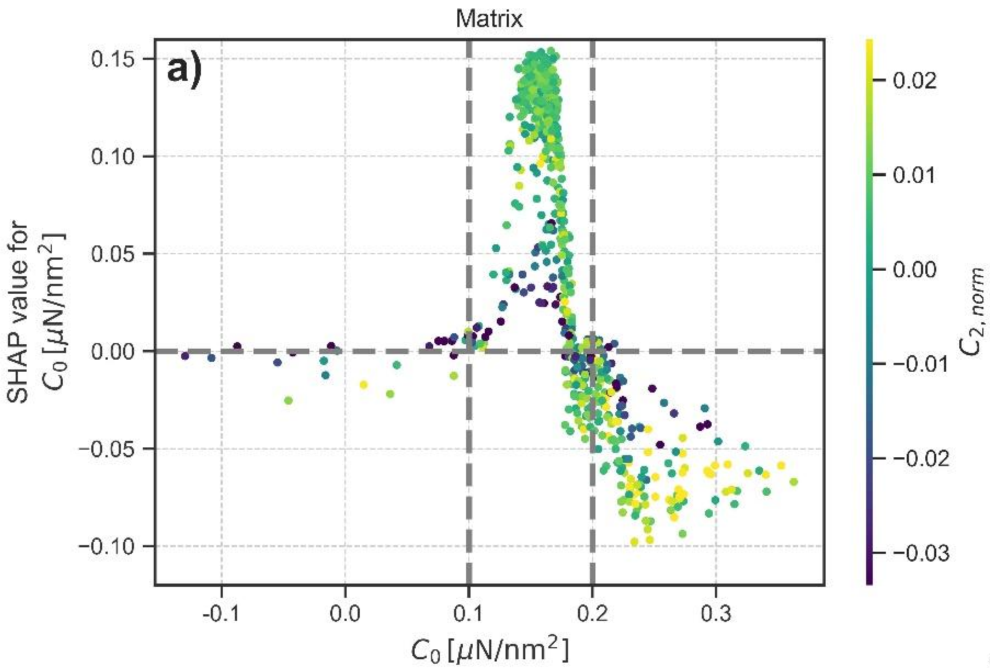


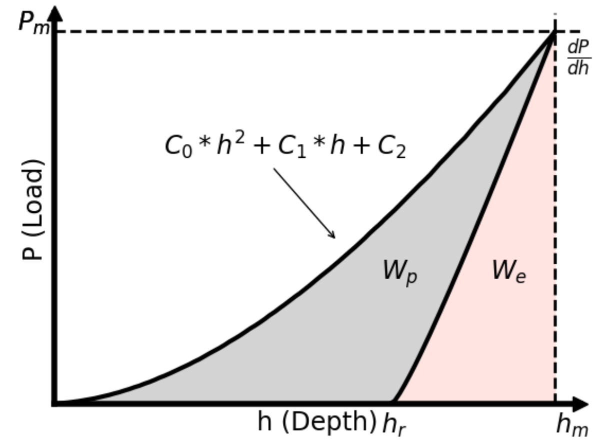
SHAP on a local level

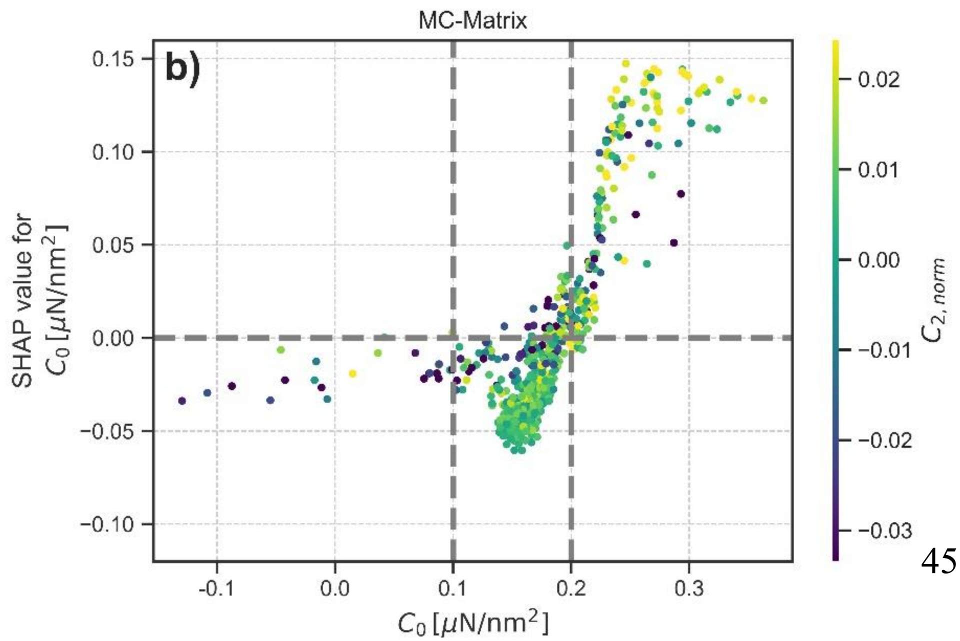




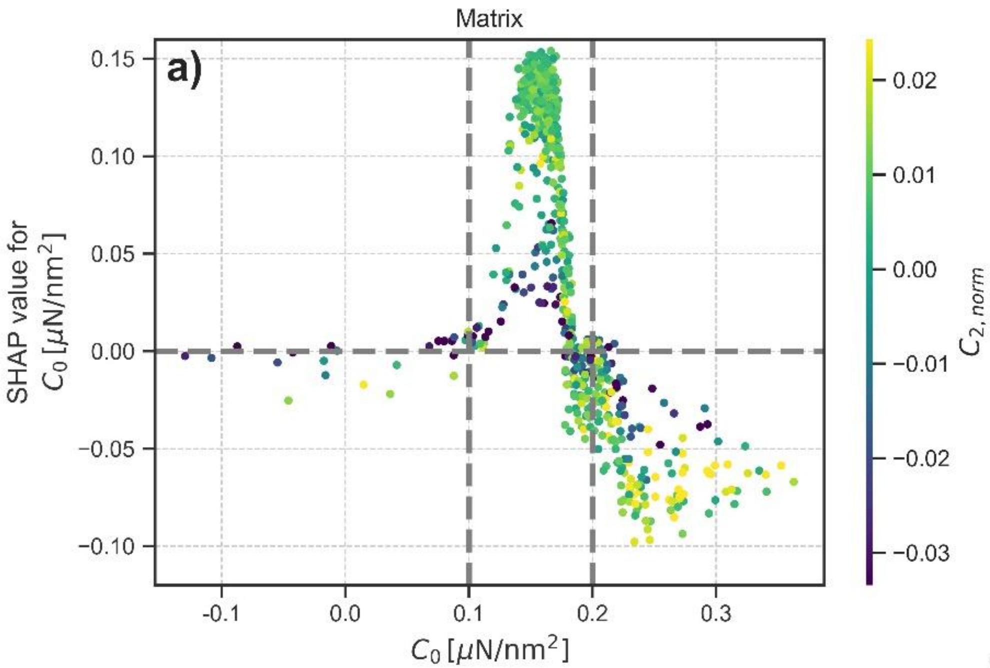
SHAP on a local level

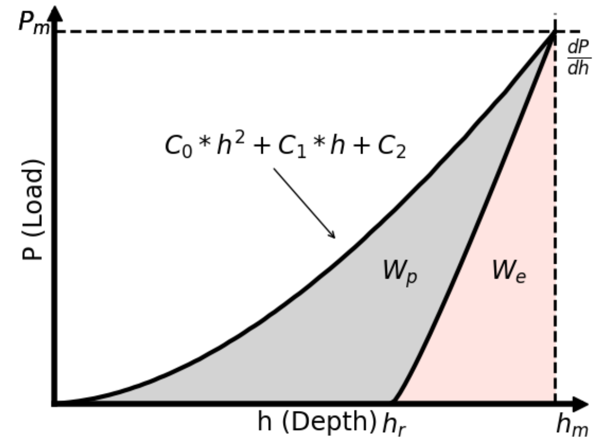


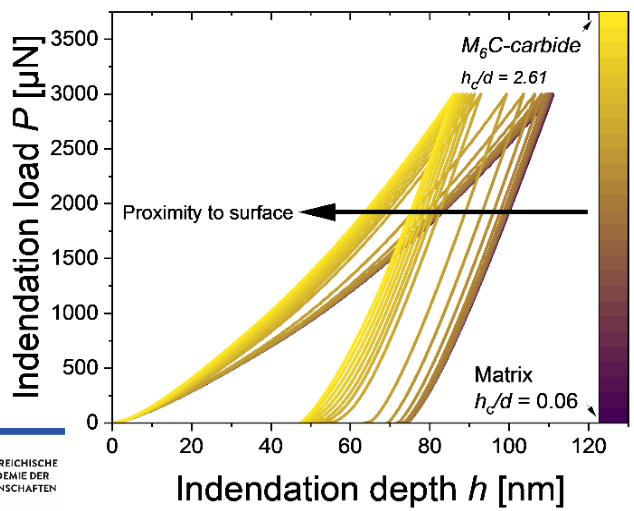


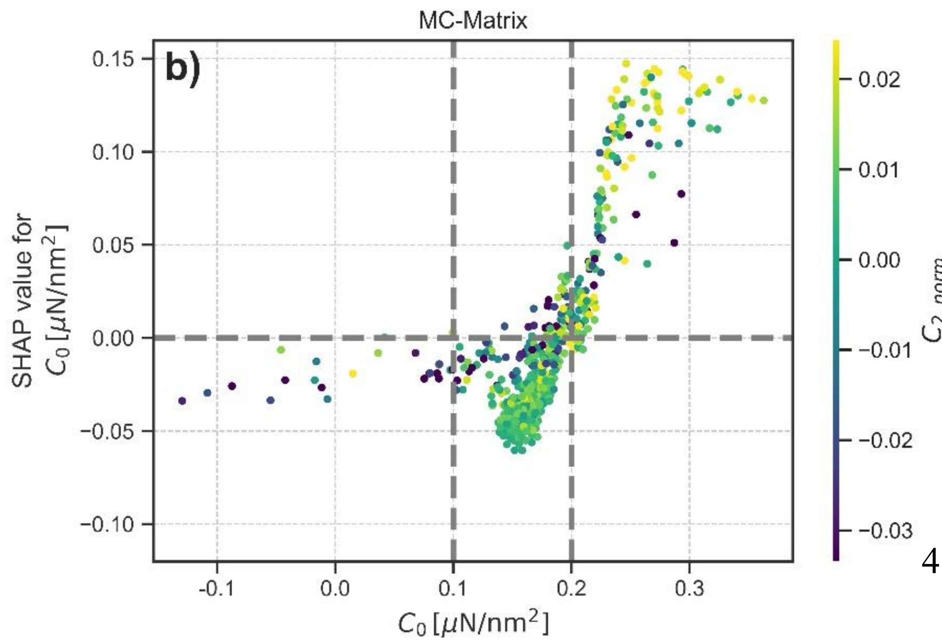


SHAP on a local level









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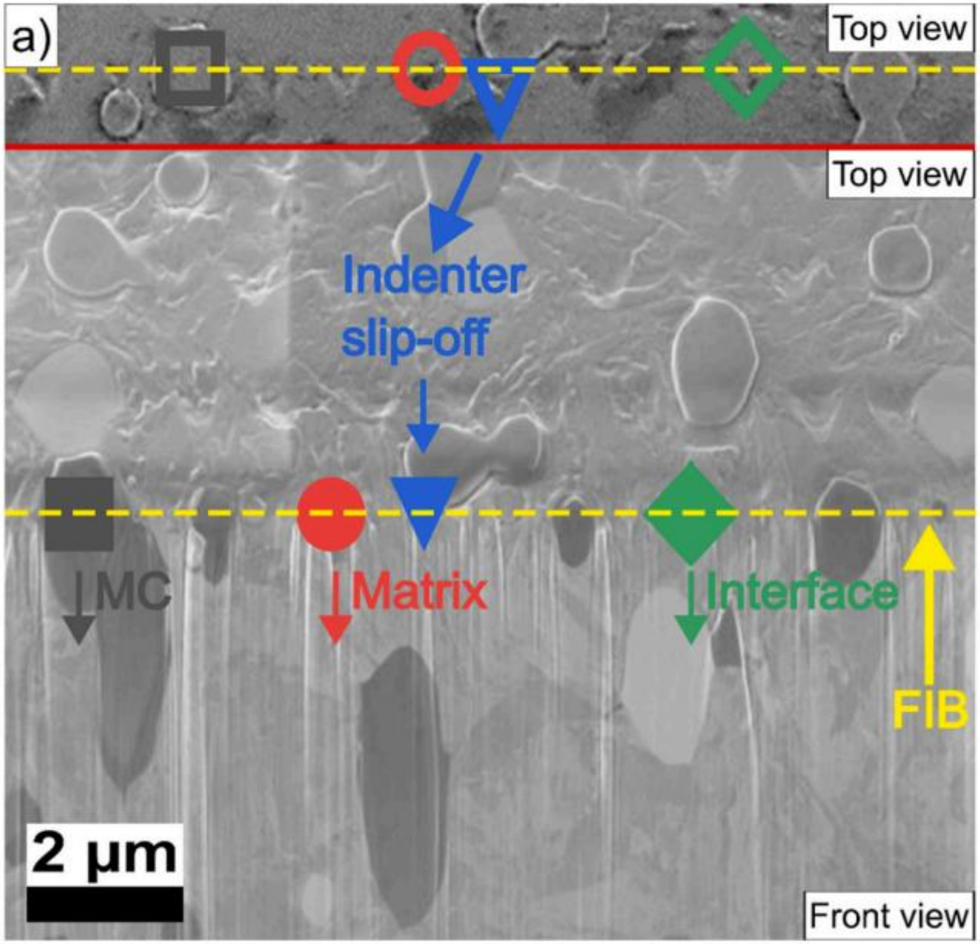
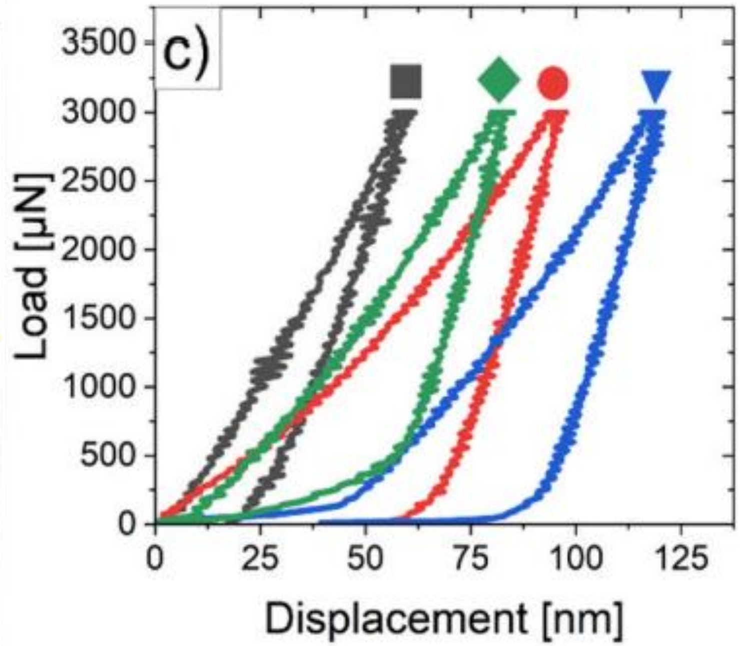
Experimental Validation





L. Walch, C. O.W. Trost, K. Kutlesa, J. Zitz, T. Klünsner, G. Ressel, A.Hackl, M. J. Cordill, S. Zak; *“**Sensing Particles Under the Surface with Nanoindentation**”*, Materials and Design, 2025, https://doi.org/10.1016/j.matdes.2025.114008

NANOINDENTATION COMBINED WITH EXPLAINABLE MACHINE LEARNING

Claus O. W. Trost[1,2]

Stanislav Žák[1]

Sebastian Schaffer[3,4]

Lukas Exl[3,4]

Megan J. Cordill[1]

[1]Erich Schmid Institute, Austrian Academy of Sciences, Leoben, Austria

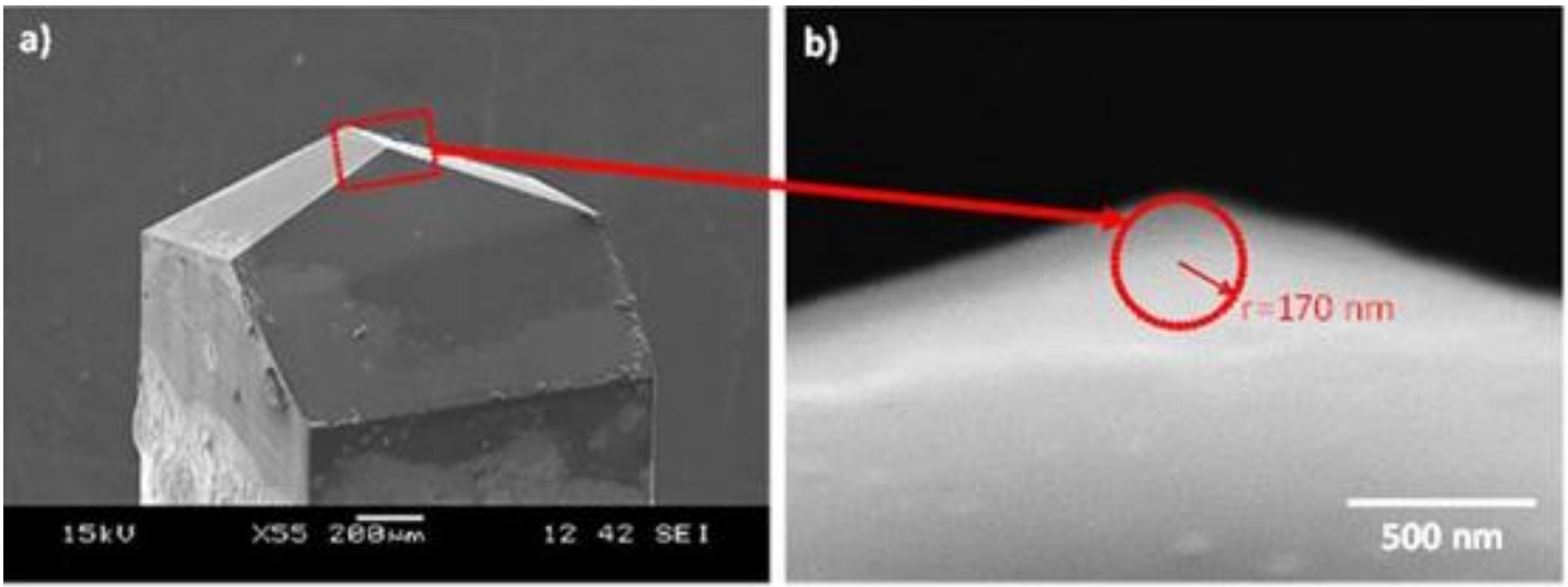
[2]Cross Disciplinary Platform for Machine Learning, Austrian Academy of Sciences, Vienna, Austria

[3]Wolfgang Pauli Institute, Faculty of Mathematics, University of Vienna, Austria.

[4]University of Vienna Research Platform MMM Mathematics - Magnetism - Materials, University of Vienna, Austria

Research Question

How sharp are our tips, and can we monitor them during high-throughput nanoindentation?



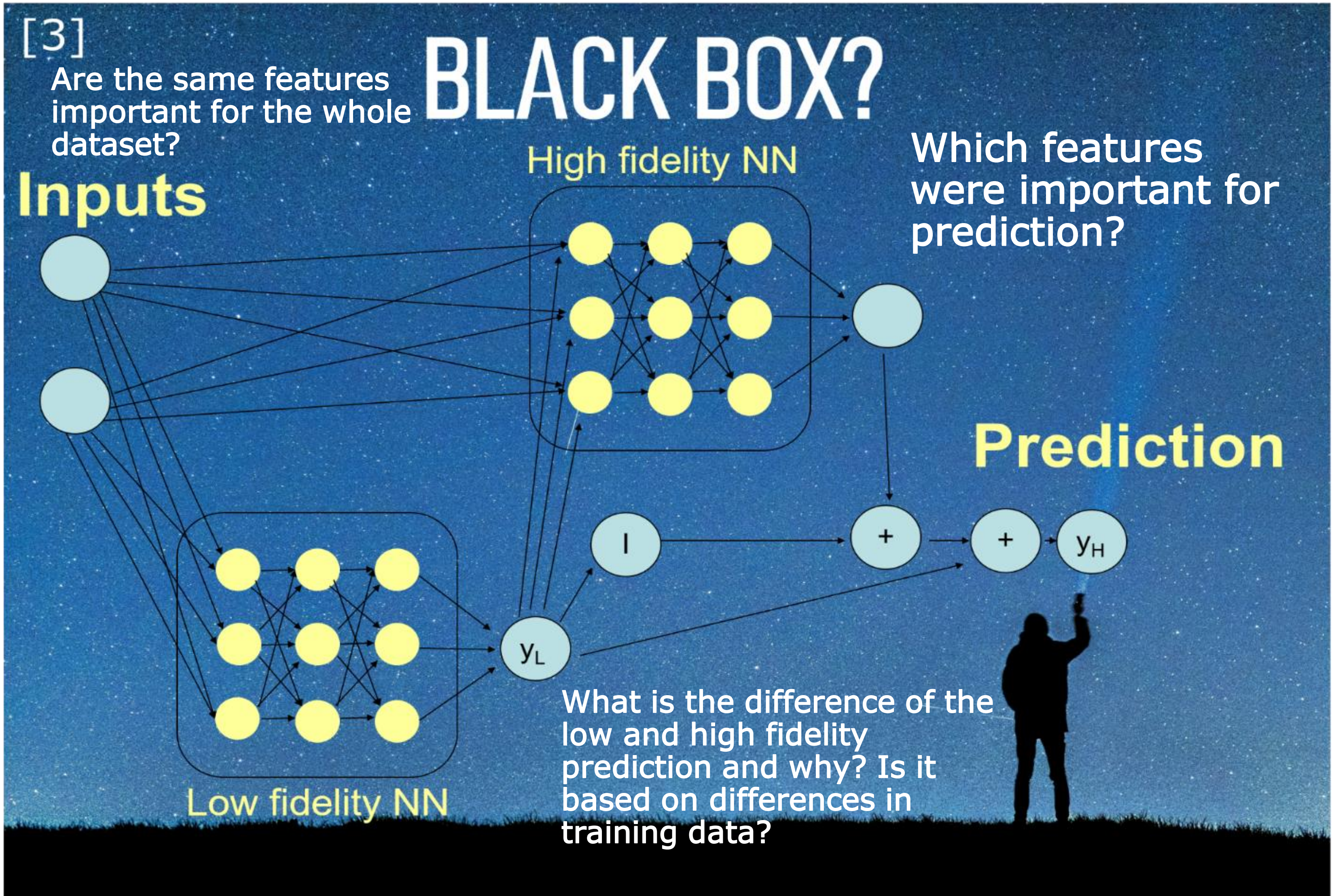
Nunez, Emerson & Bashandeh, Kian & Polycarpou, Andreas. (2020). Thermal and Mechanical Properties of Polymer Coatings. 10.1201/9780429199226-9.

Research Question

How sharp are our tips, and can we monitor them during high-throughput nanoindentation?

Why can ML models accurately predict material properties without knowing the calibration?

Machine Learning Setup



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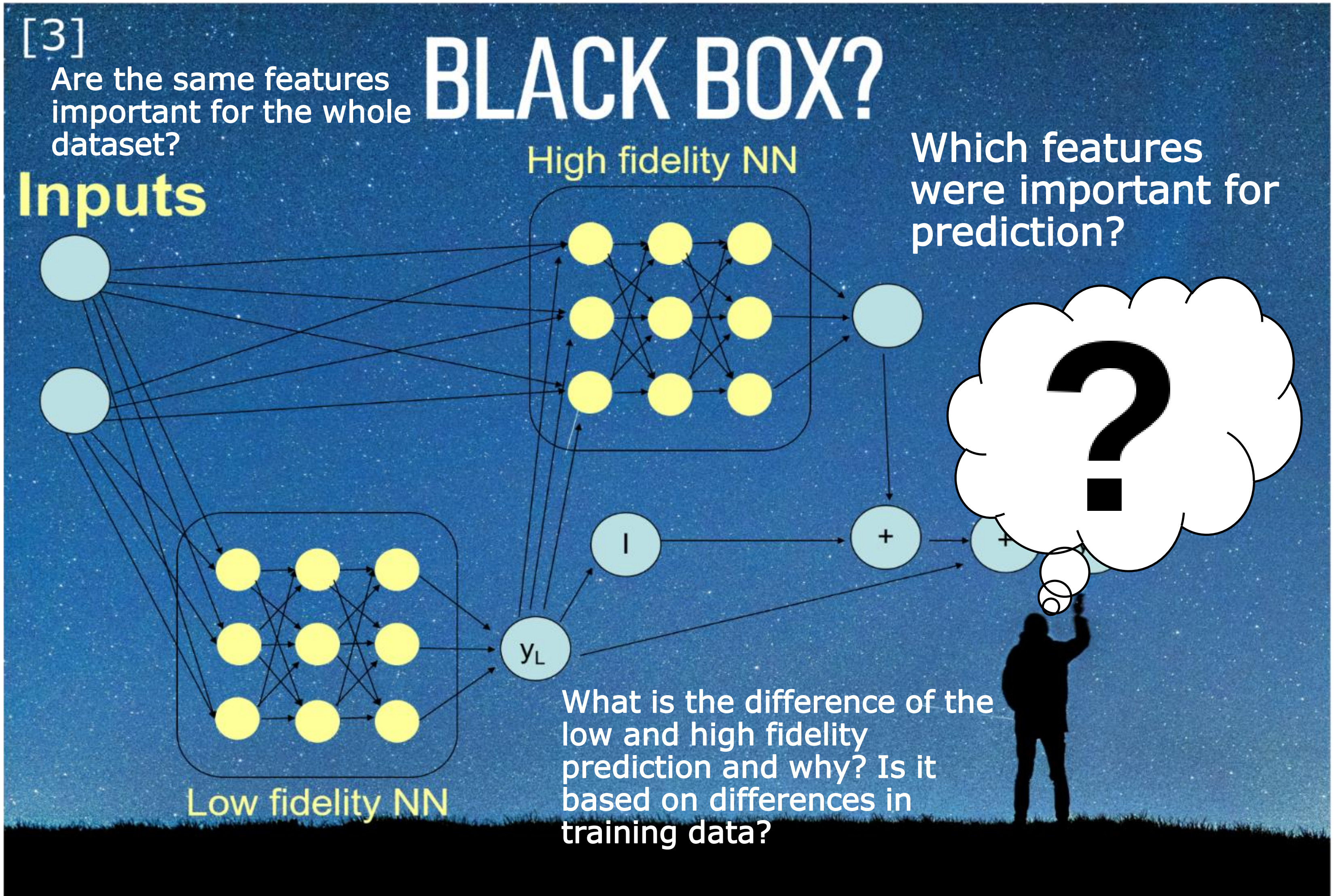
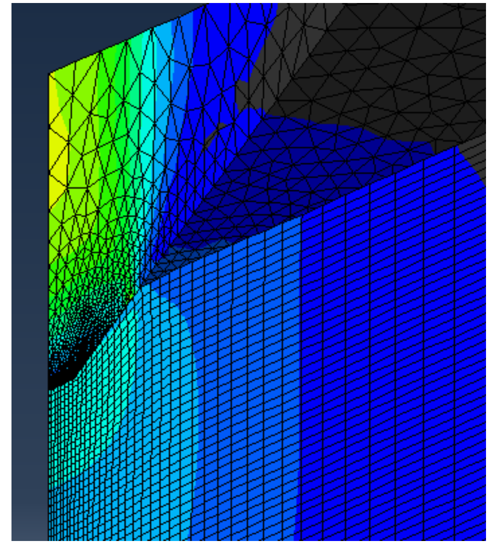


ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

E S I

Simulations

- **Abaqus – Python based Models**
- **2D and 3D Simulation incl. Tip Radius**
  - 184 2D → Sphero-Conical
  - 58 3D → Berkovich



[1] M. Dao, N. Chollacoop, K. J. van Vliet, T. A. Venkatesh, and S. Suresh, “Computational modeling of the forward and reverse problems in instrumented sharp indentation,” Acta Materialia, vol. 49, no. 19, pp. 3899–3918, 2001, doi: 10.1016/S1359-6454(01)00295-6

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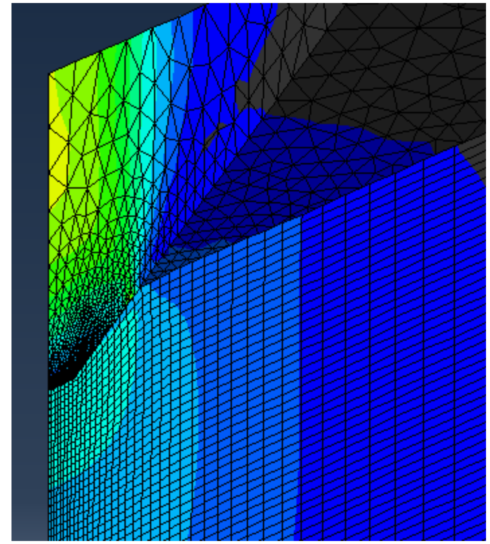


GitHub

Similar Materials space as in Dao et al.

Avoiding the realm of Mystical Materials

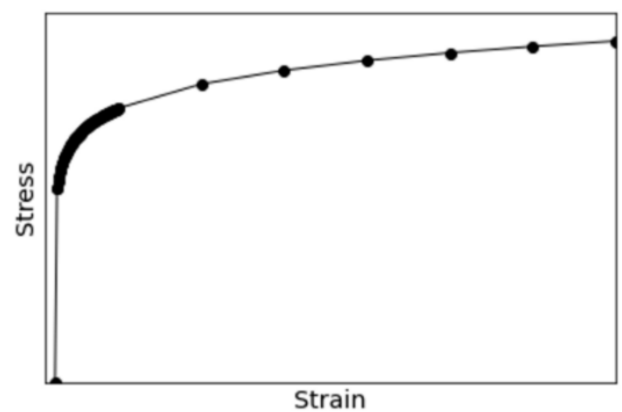
ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

[1] M. Dao, N. Chollacoop, K. J. van Vliet, T. A. Venkatesh, and S. Suresh, "Computational modeling of the forward and reverse problems in instrumented sharp indentation," Acta Materialia, vol. 49, no. 19, pp. 3899–3918, 2001, doi: 10.1016/S1359-6454(01)00295-6

E S I

Challenge → Experimental Data

- What is our ground truth?
  - <u>Simulations</u> → Simulation inputs



Challenge → Experimental Data

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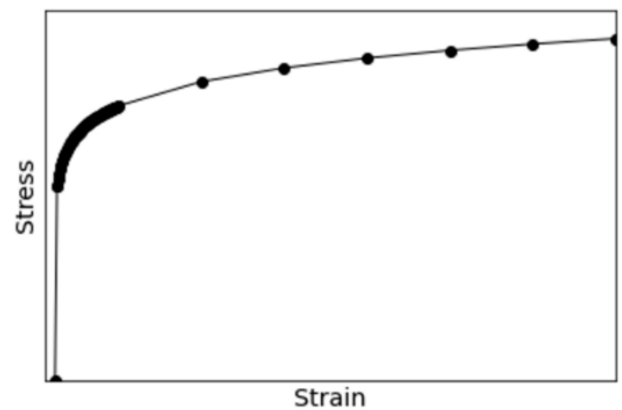
    - **Material properties (relatively easy)**



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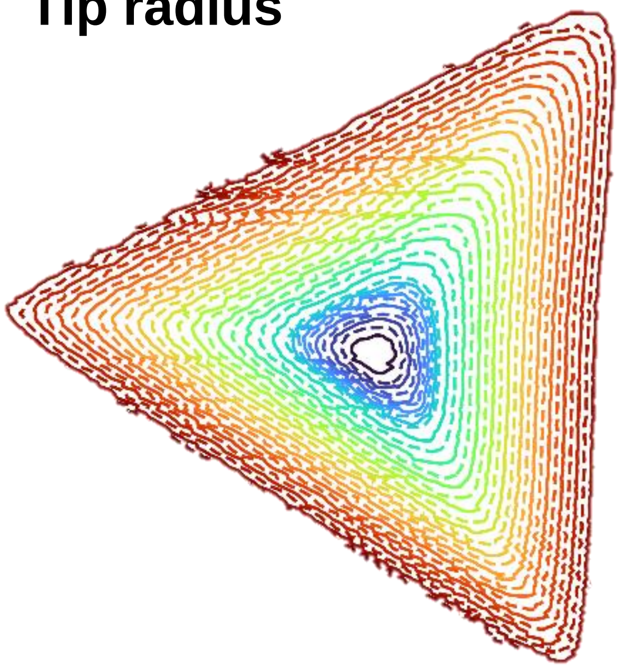
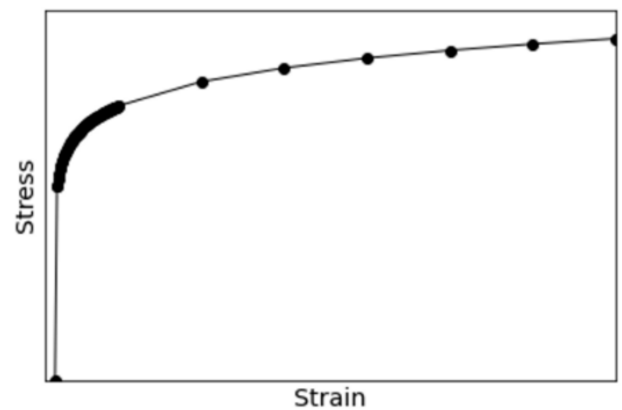
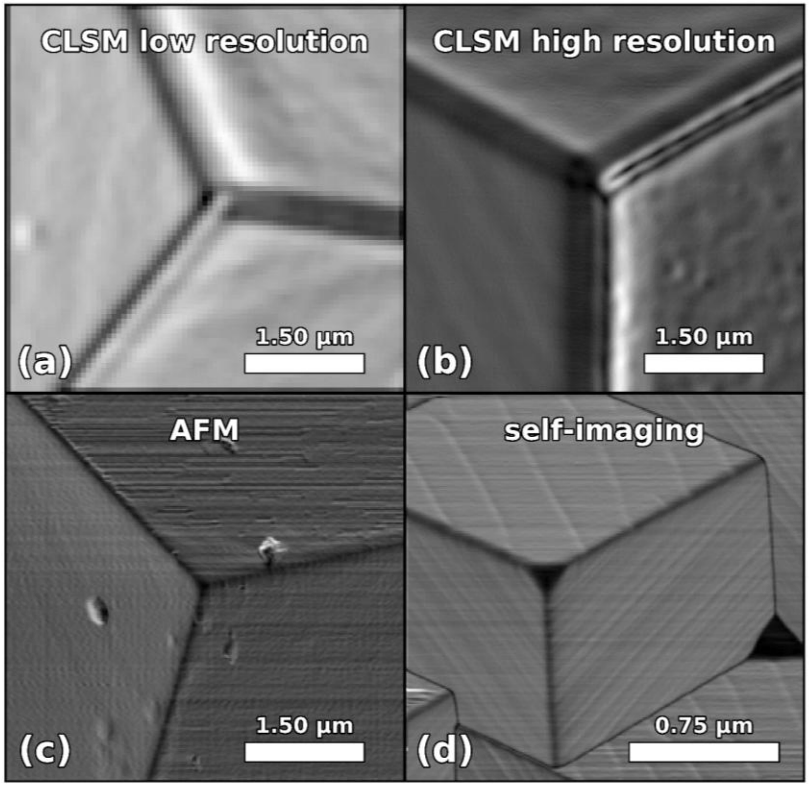




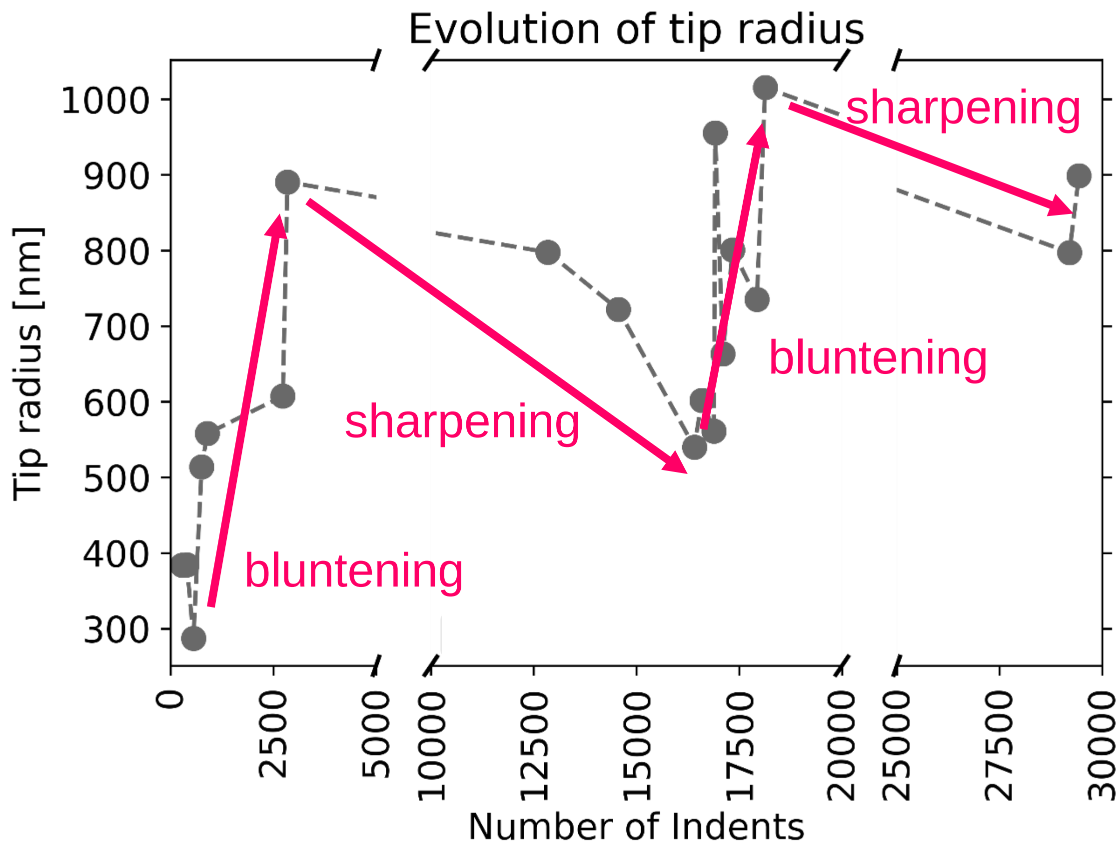
- Self imaging
  - High spatial resolution (7.8 nm in *x* & *y*)

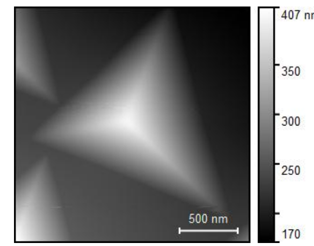


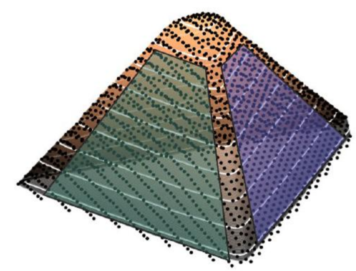
For further info see:
Saringer, C., Tkadletz, M., Kratzer, M., Cordill M. J. *et al.* **Direct determination of the area function for nanoindentation experiments**. *Journal of Materials Research* **36,** 2154–2165 (2021). https://doi.org/10.1557/s43578-021-00113-9

Tip wear experiments

- Monitoring of the tip during **30,000 indents** under actual laboratory conditions (vast amount of different materials and indentation procedures)







Wear behaviour = f(materials, number of indents, indentation procedure, scanning, ….)

ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

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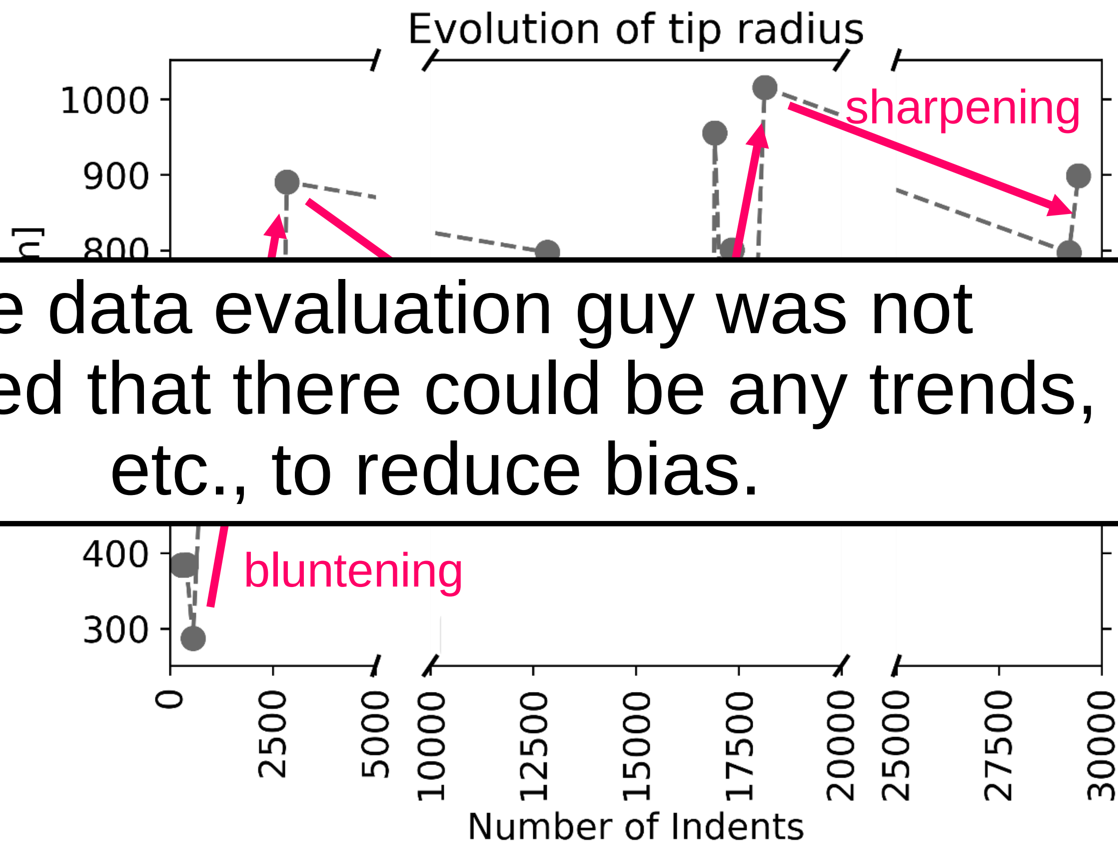
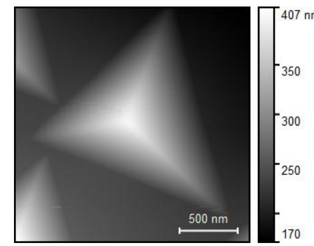
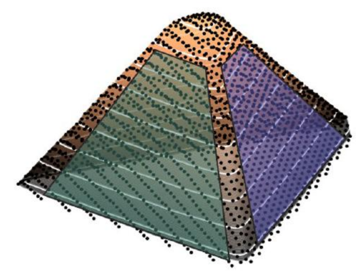


The data evaluation guy was not informed that there could be any trends, etc., to reduce bias.





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Experimental Dataset

- Assume the tip does not change 5 indents before and after the characterisation procedure

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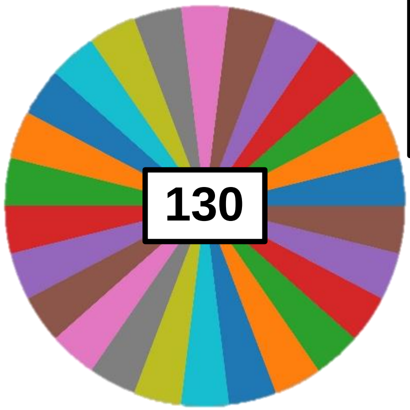
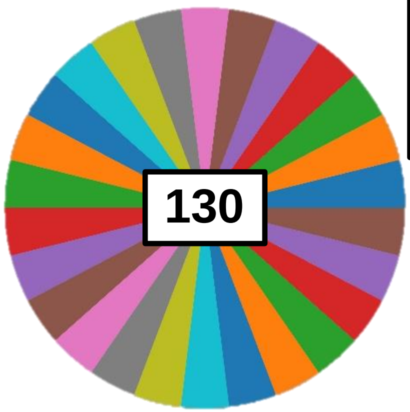


Different materials, indentation depths, tip radii

Experimental Dataset

- Assume the tip does not change <u>5 indents </u>before and after the characterisation procedure



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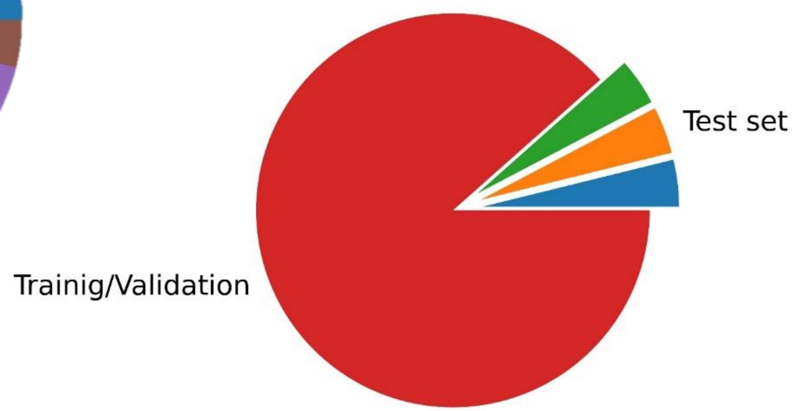
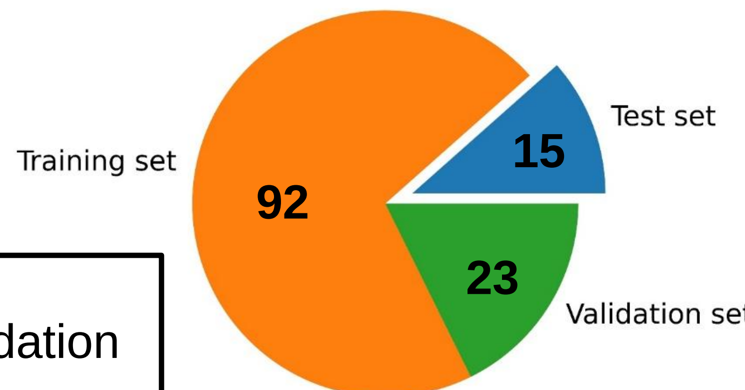


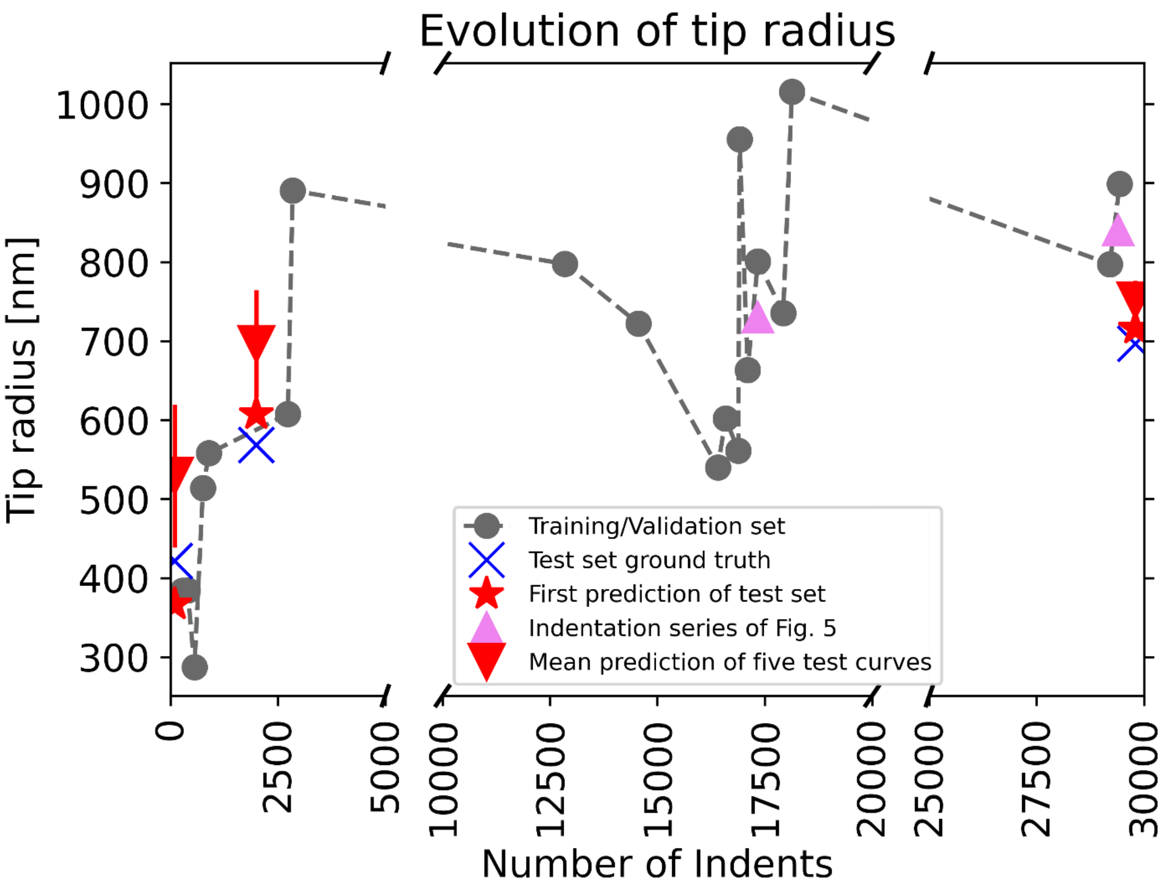
15 curves test set – 5 same material & tip radius but different indentation depth



Scrambled training/validation set

Results

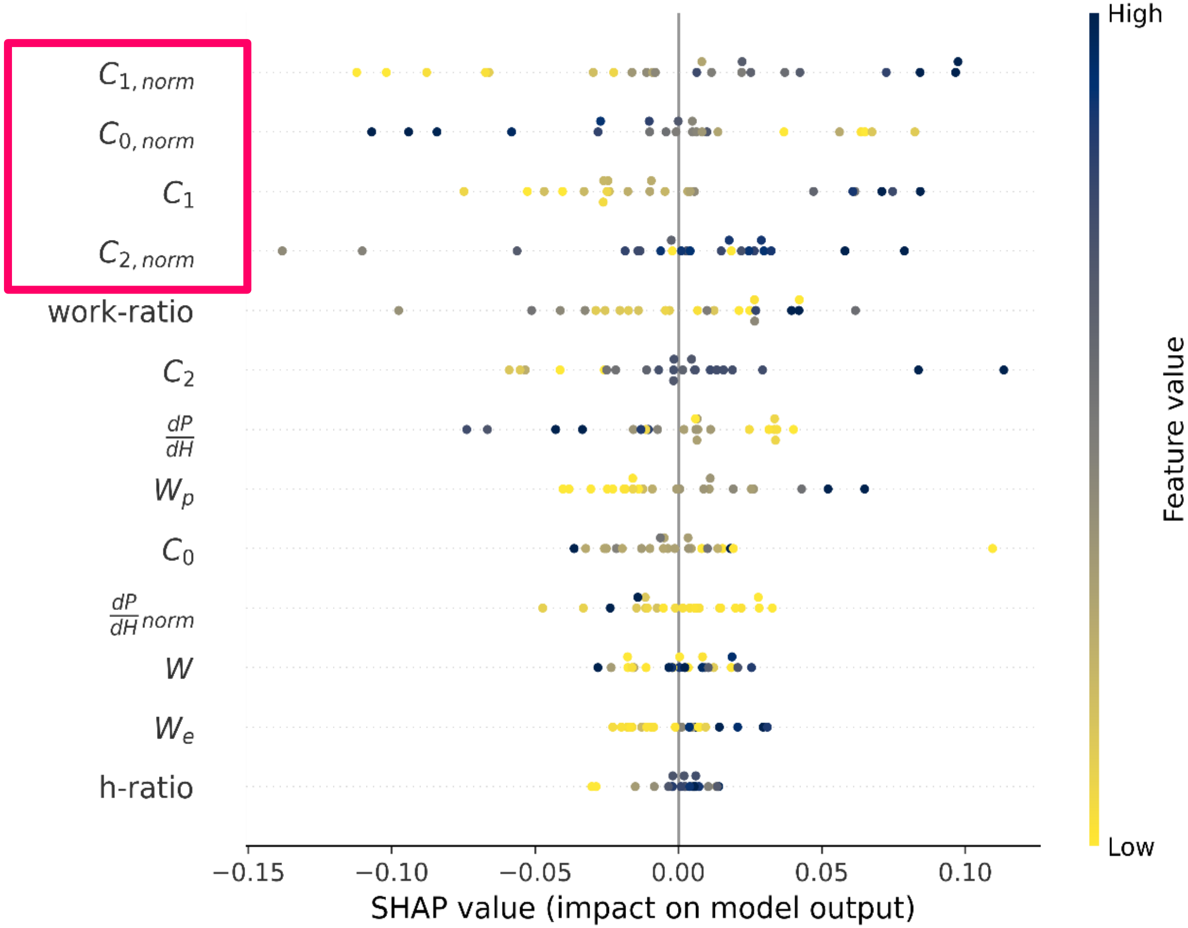
- Compare the experimental tip radii with ML



MAPE on 5-fold cross validation
12.4±3.8 MAPE

MAPE on test set
16.1 MAPE

Interpretation - Results



(Normalized-) loading curve parameters are the most important parameters!

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E S I

Journal of
MATERIALS RESEARCH

Welcome Comments Help

Further analysis of indentation loading curves: Effects of tip rounding on mechanical property measurements

Yang-Tse Cheng[a)]
Physics and Physical Chemistry Department, General Motors Global Research and Development Operations, Warren, Michigan 48090

Che-Min Cheng (Zheng Zhemin)[b)]
Laboratory for Non-linear Mechanics of Continuous Media, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

(Received 10 July 1997; accepted 15 October 1997)

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Laboratory for Non-linear Mechanics of Continuous Media, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

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$$F = c_0 h^2 + c_1 h + c_2 \,, \tag{9}$$

where the coefficient c_0 depends only on the property of materials (E, ν, Y), c_1 and c_2 are functions of tip radius and materials properties. Specifically,

$$c_0 = E\Pi(Y/E, \nu) \,, \tag{10}$$

and, using Eq. (6),

$$c_1 = 2c_0 \Delta h = 2E\Pi(Y/E, \nu)\left(\frac{1}{\sin\theta} - 1\right)R \,. \tag{11}$$

Fig. 6 shows the fits using Eq. (9) to the calculated indentation loading curves shown in Fig 4. Excellent agreements are evident for a wide range of h/R, confirming that the loading curves can be approximated by the second-order polynomials given by Eq. (9).

Table I summarizes the fitting parameters c_0/E and the tip radius, R, evaluated using Eq. (11) for three values of Y/E. The fitting parameter c_0/E agrees, to less than 3%, with that for the ideally sharp conical indenter for $h/R > 0.5$ and less than 17% for $0.25 < h/R < 0.5$ (Table I), suggesting that the parameter c_0/E is indeed relatively insensitive to the radius within the range of h/R considered. The tip radius, R, evaluated

R_{mod} (μm)	R (μm)	c_0/E	R (μm)	c_0/E	R (μm)	c_0/E
0.00	0.0	1.66	0.0	0.59	0.0	0.28
0.25	0.18	1.68	0.21	0.58	0.20	0.28
0.50	0.44	1.68	0.46	0.58	0.51	0.28
1.00	1.1	1.62	1.1	0.57	1.1	0.27
2.00	3.3	1.42	3.0	0.50	3.1	0.24

using Eq. (11), also approximately agrees with that given to the finite element models (Table I).

Based on the above analysis, we propose a new method for determining yield strength, Y, and indenter tip radius, R, using indentation loading curves together with known E and ν:

(1) Experimental loading curve is fitted with a second-order polynomial, Eq. (9), and the coefficients, c_0 and c_1, are determined.

(2) Divide c_0 by E and obtain $\Pi\,(Y/E, \nu) \approx c_0/E$.

(3) Determine Y/E, and consequently Y, using the scaling relationship $\Pi\,(Y/E, \nu)$ given by Fig. 2 or from the approximate scaling relationship $(1 - \nu^2)\Pi^*$ (Y/E) given by Fig. 3 together with either a known or representative value for ν.

(4) Determine the tip radius using c_0, c_1, and Eq. (11), i.e., $R = c_1/[2c_0(1/\sin\theta - 1)]$.

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Further analysis of indentation loading curves: Effects of tip rounding on mechanical property measurements

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(Received 10 July 1997; accepted 15 October 1997)

$$F = c_0 h^2 + c_1 h + c_2 \,, \qquad (9)$$

where the coefficient c_0 depends only on the property of materials (E, ν, Y), c_1 and c_2 are functions of tip radius and materials properties. Specifically,

$$c_0 = E\Pi(Y/E, \nu) \,, \qquad (10)$$

and, using Eq. (6),

$$c_1 = 2c_0 \Delta h = 2E\Pi(Y/E, \nu)\left(\frac{1}{\sin\theta} - 1\right)R \,. \qquad (11)$$

Fig. 6 shows the fits using Eq. (9) to the calculated indentation loading curves shown in Fig 4. Excellent agreements are evident for a wide range of h/R, co… firming that the loading curves can be approximated b… the second-order polynomials given by Eq. (9).

Table I summarizes the fitting parameters c_0/E and the tip radius, R, evaluated using Eq. (11) for three values of Y/E. The fitting parameter c_0/E agrees, to less than 3%, with that for the ideally sharp conical indenter for $h/R > 0.5$ and less than 17% for $0.25 < h/R < 0.5$ (Table I), suggesting that the parameter c_0/E is indeed relatively insensitive to the radius within the range of h/R considered. The tip radius, R, evaluated

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Bas… …ropose a new met… …n, Y, and indenter … …oading curves together …

… …oading curve is fitted with a … …omial, Eq. (9), and the coefficients, … determined.

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(4) Determine the tip radius using c_0, c_1, and Eq. (11), i.e., $R = c_1/[2c_0(1/\sin\theta - 1)]$.

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Inverse identification of constitutive parameters with instrumented indentation test considering the normalized loading and unloading *P-h* curves

Yu Gang Li[a,*], Pascale Kanouté[b,c], Manuel François[b], Dong Chen[a,*], Hao Wei Wang[a]

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[b] ICD-LASMIS, UMR CNRS 6281, Université de Technologie de Troyes (UTT), 12, rue Marie Curie - CS 42060, 10010 Troyes Cedex, France
[c] The French Aerospace Lab (ONERA), DMSM/MCE, 29 avenue de la Division Leclerc-BP 72, F-92322 Chatillon Cedex, France

Inverse identification of constitutive parameters with instrumented indentation test considering the normalized loading and unloading *P-h* curves

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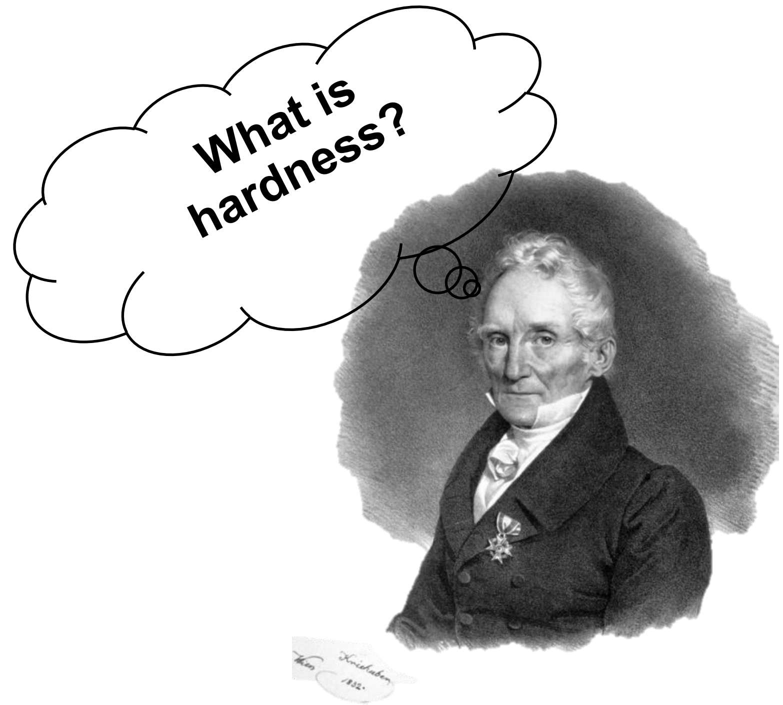
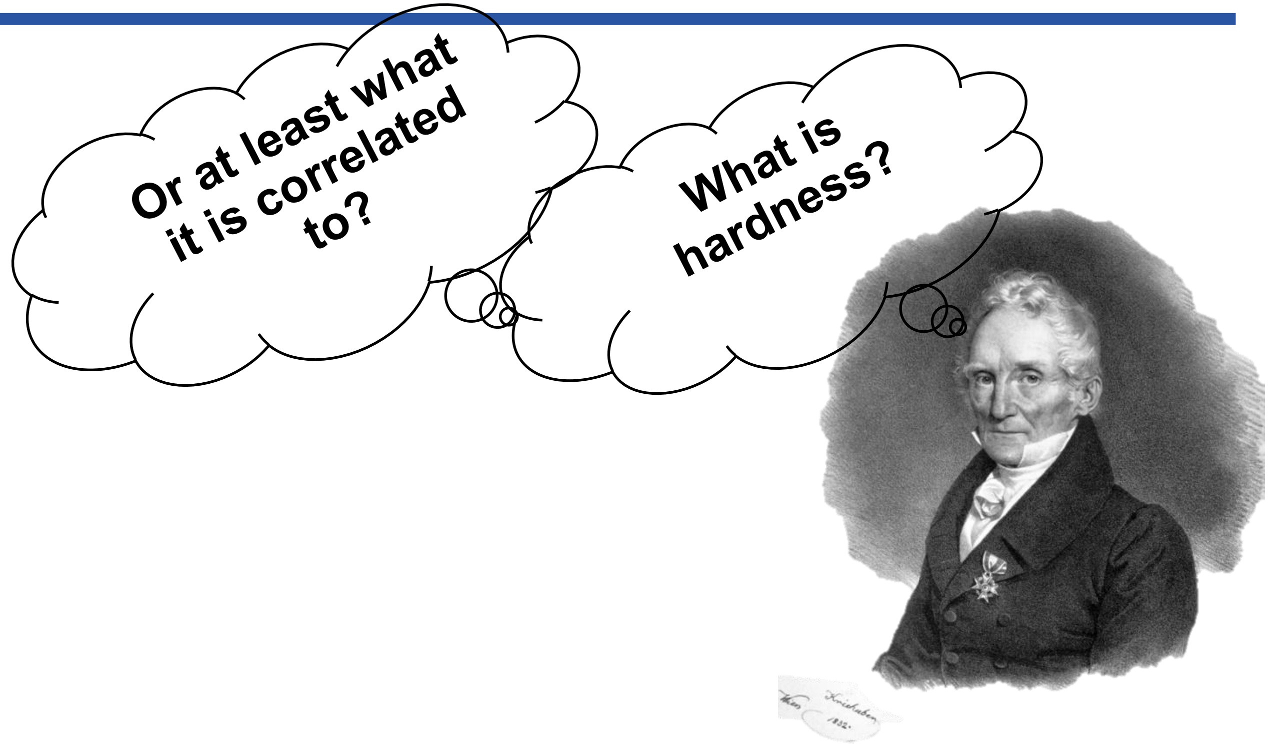
this.

In the present study, theoretical analysis based on the well-known Kick's law showed that the shape of the normalized loading *P-h* curve is highly correlated with the tip rounding radius. Further sophisticated numerical sensitivity analysis has confirmed this, which means that the shape of the normalized loading *P-h* curve can be used for the tip rounding calibration.



USING NANOINDENTATION LITERATURE DATA TO FIND NOVEL SUPER HARD MATERIALS



USING NANOINDENTATION LITERATURE DATA TO FIND NOVEL SUPER HARD MATERIALS

Dataset

Zhang, Z.; Mansouri Tehrani, A.; Oliynyk, A. O.; Day, B.; Brgoch, J. Finding the next superhard material through ensemble learning. Adv. Mater. 2021, 33, 2005112
Russlan Jaafreh, Yoo Seong Kang, Jung-Gu Kim, Kotiba Hamad, Machine learning guided discovery of super-hard high entropy ceramics, Materials Letters, Volume 306, 2022, https://doi.org/10.1016/j.matlet.2021.130899.
Zhang, Z et. al.; Determining Temperature-Dependent Vickers Hardness with Machine Learning, The Journal of Physical Chemistry Letters, doi: 10.1021/acs.jpclett.1c01845

	Composition	avg_ Atomic_Number	avg_ Atomic_Weight	avg_Period	avg_group	avg_families	avg_Mendeleev Number	avg_Atomic Radus
0	Ag0.05Gd0.048Pd0.902	46.914	108.93225	5.048	9.714	3.952	60.47	1.4292
1	Ag0.05Y0.048Pd0.902	45.714	105.651731	5.0	9.714	3.952	59.75	1.4292
2	Ag0.25Pb0.5Sb0.25Te	58.75	144.303525	5.25	14.75	5.5	84.0	1.53125
3	Al1.5Si1.5N2.5O1.5					43	80.285714	0.864286
4	Al1.67B22					47	72.070553	0.878221
...	...					...	...	...
2146	ZrAlMo					33	55.666667	1.416667
2147	ThAl2Fe3	32.333333	75.590363	4.166667	8.833333	4.166667	54.5	1.416667
2148	LaMnNi4	32.333333	71.436192	4.333333	8.333333	3.833333	51.5	1.458333
2149	LaMgAl11O19	11.375	23.874876	2.5	14.125	6.03125	79.28125	0.89375
2150	Al3BC3	8.857143	18.255517	2.428571	13.428571	6.0	74.571429	0.957143

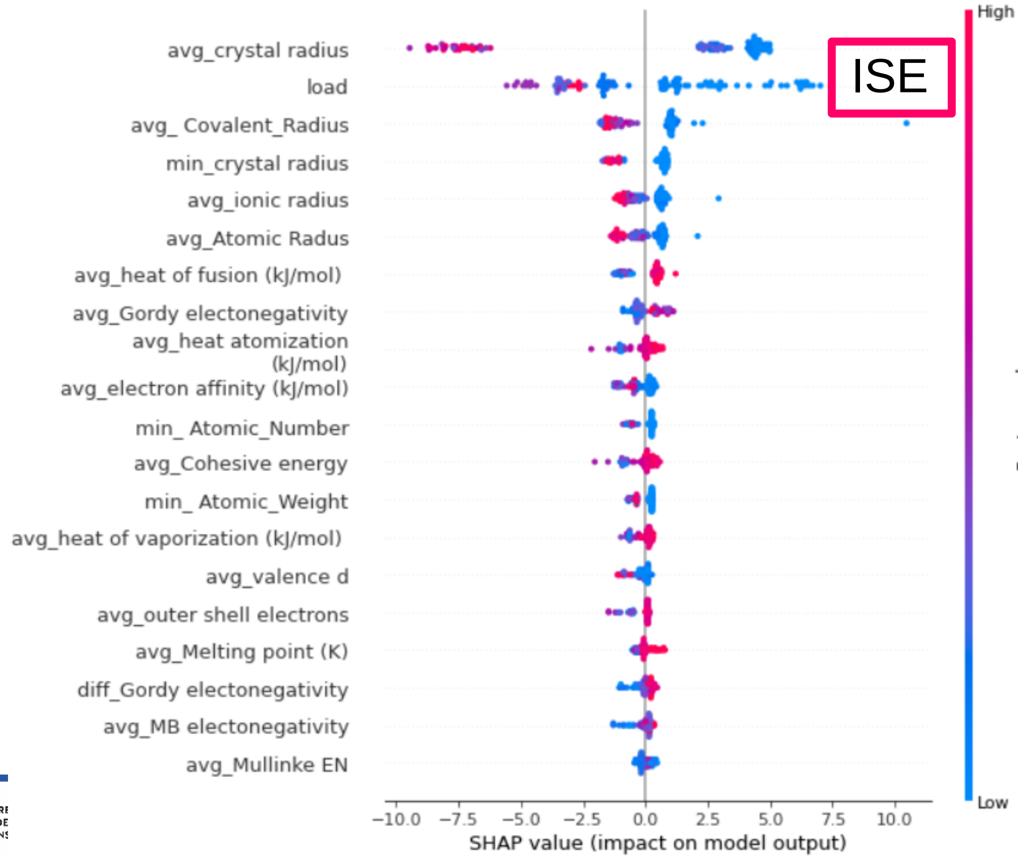
Combined datasets, dropped duplicates

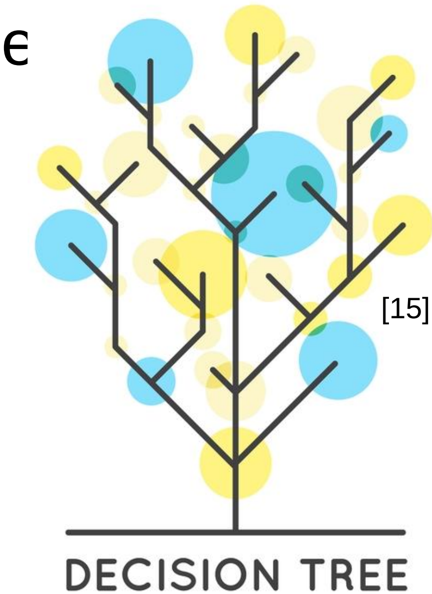
2151 rows × 143 columns

141 features –> 35 compositional descriptions combined with mathematical expressions

Predicting Hardness

- Zhang et al. trained tree based XGBoost [13] model to **predict Vickers hardness** with 35 compositional descriptions combined with mathematical e
  - **Total 141 features (including load)**
  - **< 2 minutes calculation time on a laptop!**





[15]

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How do I publish my data?

Roche DG, Lanfear R, Binning SA, Haff TM, Schwanz LE, et al. (2014) Troubleshooting Public Data Archiving: Suggestions to Increase Participation. PLoS Biol 12(1): e1001779. doi:10.1371/journal.pbio.1001779

ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

Publishing Data

Published June 11, 2025 | Version v1

Dataset | Open

The High-Speed Steel S390 Microclean™ Nanoindentation Dataset

Trost, Claus Othmar Wolfgang (Data manager)[1]; Žák, Stanislav (Data collector)[1]; Walch, Lukas (Annotator)[2]; Zitz, Jakob (Annotator)[2]; Cordill, Megan J. (Data curator)

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Contributors

Researcher (7):

Trost, Claus Othmar Wolfgang[1]; Žák, Stanislav[1]; Schaffer, Sebastian[2]; Klünsner, Thomas[3]; Leitner, Harald[4]; Exl, Lukas[2]; Cordill, Megan J.

Show affiliations

Dataset to the paper "Explainable machine learning and feature engineering applied to nanoindentation data" https://doi.org/10.1016/j.matdes.2025.113897 published in Materials and Design.

All data was obtained from the high-speed steel (HSS) grade traded as S390 Microclean™ by voestalpine Böhler Edelstahl GmbH & Co KG. The steel was heat-treated in different ways to achieve different microstructural states. The data was measured using a TS77 Select Bruker-Hysitron Nanoindenter.

Versions

Version v1 — Jun 11, 2025

10.5281/zenodo.15639082

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Dataset Open

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Contributors

Researchers:

Trost, Clau... ...affer, Sebastian[2];

Klün... ...Cordill, Megan J.

Nanoindentation Classification & Clustering Benchmark Dataset

...ature engineering applied to nanoindentation

j.n... ...Design.

All dat... ...el (HSS) grade traded as S390 Microclean^{TM} by voestalpi

Co KG. ... ...erent ways to achieve different microstructural states. The data

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Nanoindentation - Classification of High-Speed-Steel

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PAPER

An explainable study of adaptive neuro-fuzzy inference system for spherical indentation hardness identification

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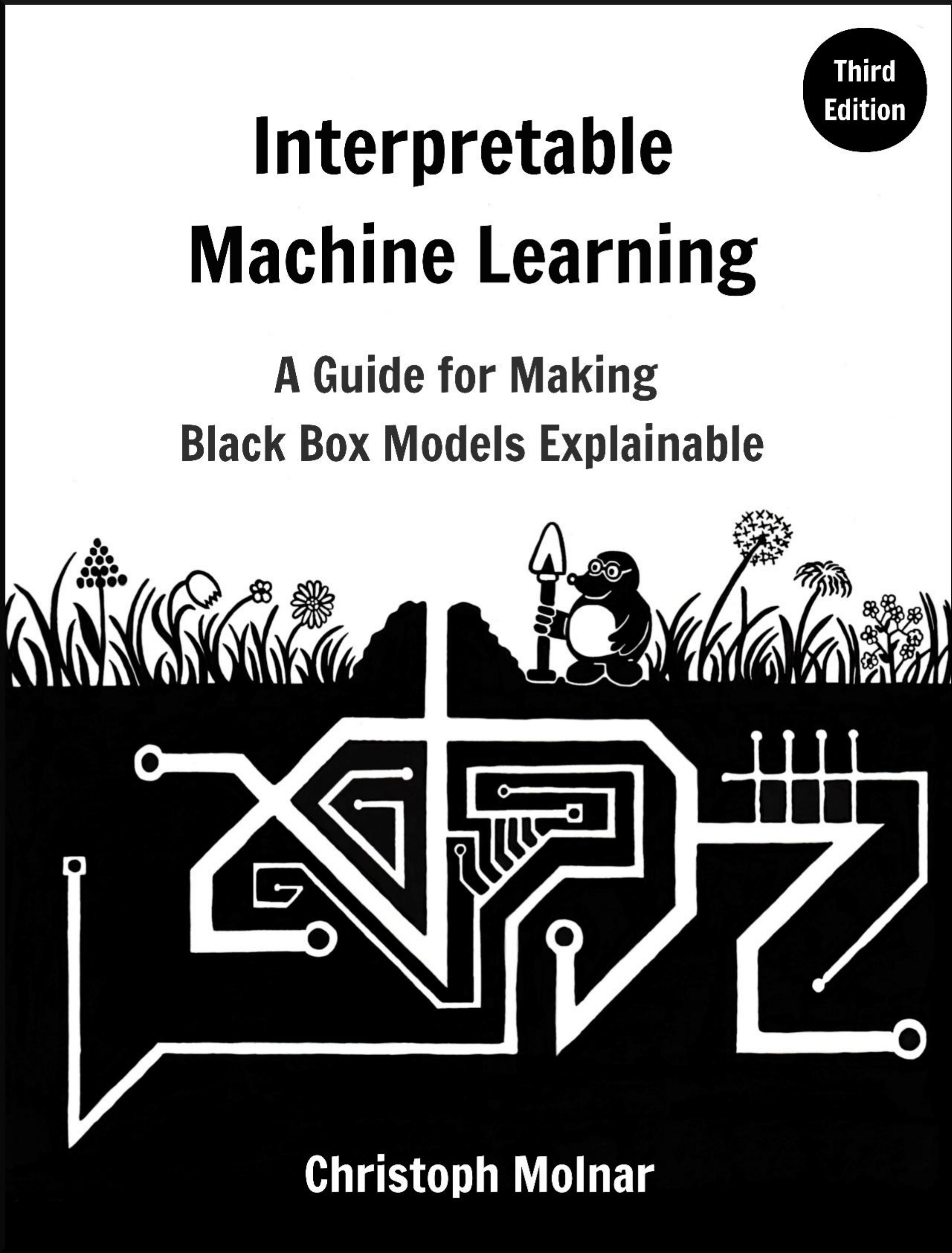
Keywords: ANFIS, indentation hardness, explainable, quality score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