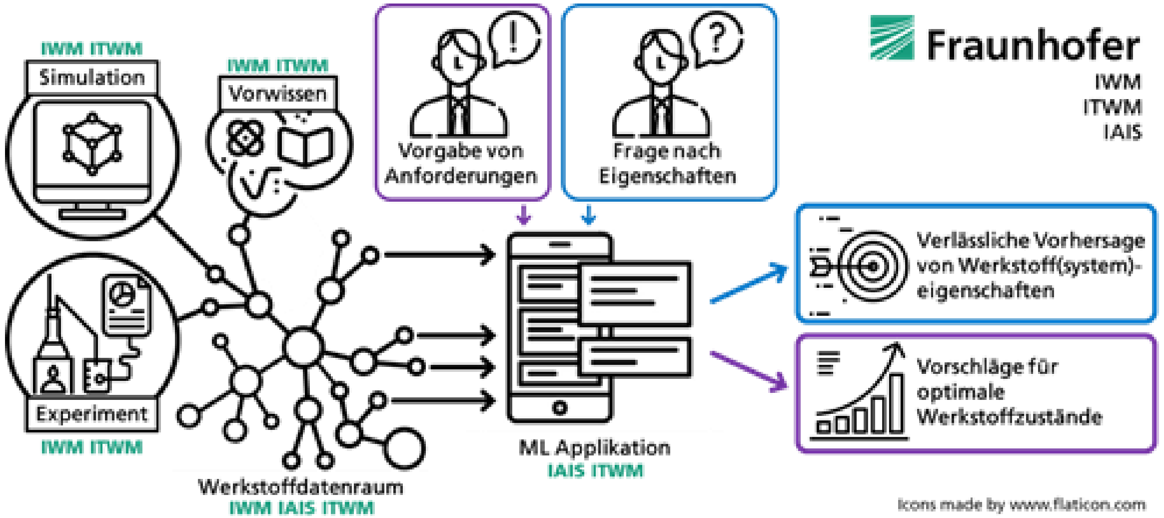
ONLINE-VERANSTALTUNG

Live-Demo Machine Learning Tool

Abschlusskolloquium
des Fraunhofer-Konsortiums »UrWerk«
zur Entwicklung von unternehmensspezifischen Werkstoff(system)-Datenräumen



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Projektleiter »UrWerk«
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am Fraunhofer-Institut für Werkstoffmechanik IWM

24.November 2022

Projekt UrWerk: Digitale Methoden für die Lebensdauerbewertung am Beispiel hochfester Stähle

LIVE-DEMO MACHINE LEARNING TOOL

24.11.2022

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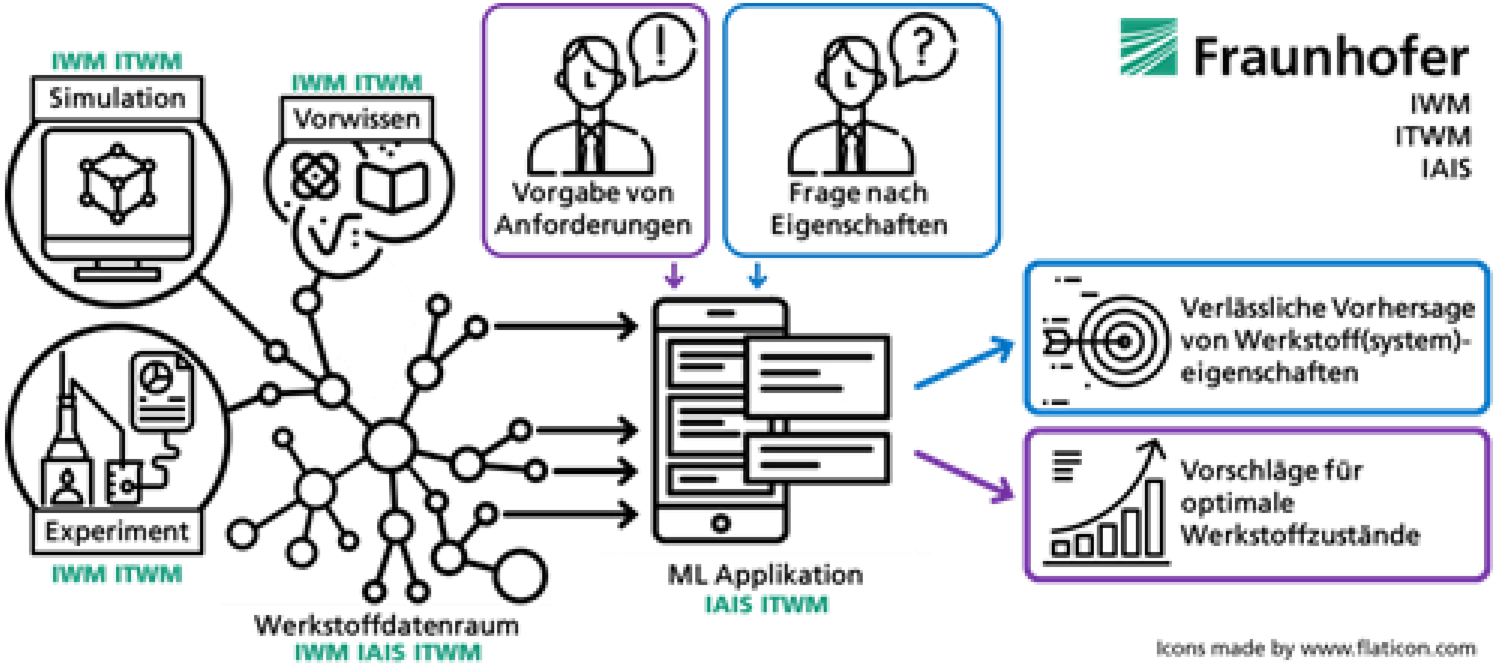

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Data Analytics / Machine Learning

Live-Demo Machine Learning Tool

- **Story 1: Hardness prediction for steels** depending on their chemical composition
  - Validation of material science knowledge (see table*)with a „real“ database
  - Aim: Establish confidence in the analysis method
- **Story 2: Fatigue strength prediction for high strength steels**
  - Industrial use case
  - Influence of chemical elements, hardness, roughness and other parameters

*Quelle: Vorlesung „Metallische Werkstoffe“, Ernst Fleischmann, Universität Bayreuth

Übersicht: Einfluß der Legierungselemente auf die Eigenschaften des Stahls

Legierungs-element		Mechanische Eigenschaften																Magnet.Eigensch.				
		Härte	Festigkeit	Streck-grenze	Dehnung	Einschnürung	Kerbschlag-zähigkeit	Elastizität	Warm-festigkeit	Abkühlge-schwindigkeit	Karbid-bildung	Verschleiß-festigkeit	Schmied-barkeit	Zerspan-barkeit	Verzunderung	Nitrier-barkeit	Rostbe-ständigkeit	Hysteresis	Permeabilität	Koerzitivkraft	Remanenz	el. Leistungs-verlust
Si		↑	↑	↑↑	↓	~	↓	↑↑↑	↑	↓	↓	↓↓↓	↓	↓	↓	↓	–	↓↓	↑↑	↓↓	–	↓↓
Mn	In perlit. Stählen	↑	↑	↑	~	~	~	↑	~	↓	~	↓↓	↑	↓	~	~	–					
Mn	In austenit. Stählen	↓↓↓	↑	↓	↑↑↑	~	–	–	–	↓↓	–	–	↓↓↓	↓↓↓	↓↓	–	–	unmagnetisch not magnetic non magnétique				
Cr		↑↑	↑↑	↑↑	↓	↓	↓	↑	↑	↓↓↓	↑↑	↑	↓	–	↓↓↓	↑↑	↑↑↑			↑	↑↑	
Ni	In perlit. Stählen	↑	↑	↑	~	~	~	–	↑	↓↓	–	↓↓	↓	↓	↓	–	–			↑↑	↑↑	
Ni	In austenit. Stählen	↓↓	↑	↓	↑↑↑	↑↑	↑↑↑	–	↑↑↑	↓↓	–	–	↓↓↓	↓↓↓	↓↓	–	↑↑	unmagnetisch not magnetic non magnétique				
Al		–	–	–	–	↓	↓	–	–	–	–	–	↓↓	–	↓↓	↑↑↑	–			↑↑	↑↑	
W		↑	↑	↑	↓	↓	~	–	↑↑↑	↓↓	↑↑	↑↑↑	↓↓	↓↓	↓↓	↑	–			↑↑↑	↑↑↑	
V		↑	↑	↑	~	~	↑	↑	↑↑	↓↓	↑↑↑↑	↑↑	↑	–	↓	↑	↑					
Co		↑	↑	↑	↓	↓	↓	–	↑↑	↑↑	–	↑↑↑	↓	~	↓	–	–		↑↑	↑↑↑	↑↑↑	
Mo		↑	↑	↑	↓	↓	↑	–	↑↑	↓↓	↑↑↑	↑↑	↓	↓	↑↑	↑↑	–			↑		
Cu		↑	↑	↑↑	~	~	~	–	↑	–	–	–	↓↓↓	~	~	–	↑					
S		–	–	–	↓	↓	↓	–	–	–	–	–	↓↓↓	↑↑↑	–	–	↓					
P		↑	↑	↑	↓	↓	↓↓↓	–	–	–	–	–	↓	↑↑	–	–	–					

↑ Erhöhung ↓ Erniedrigung ~ gleichbleibend - nicht charakteristisch oder unbekannt Mehrere Pfeile = verstärkte Wirkung

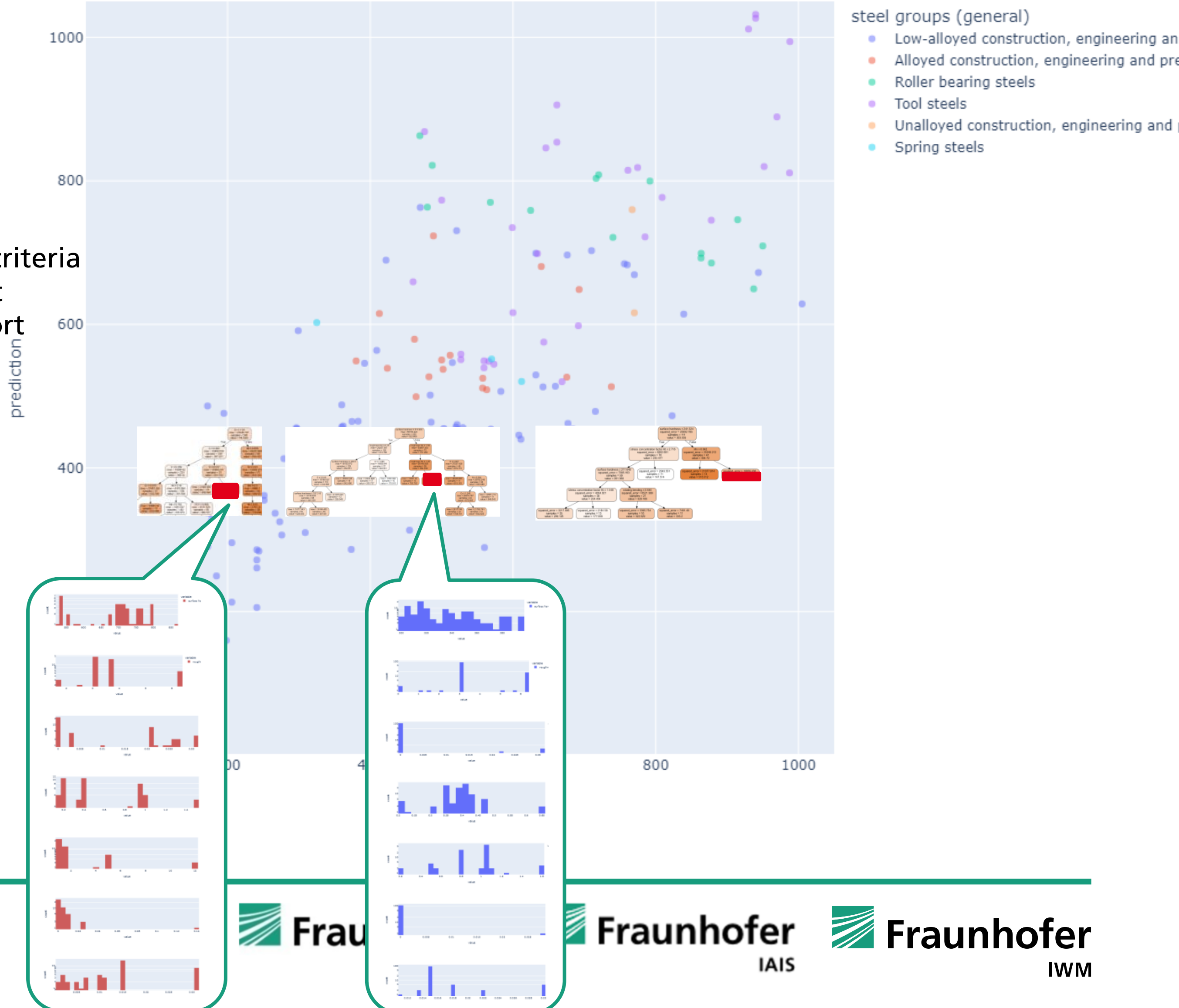
Ernst Fleischmann, Metallische Werkstoffe 138 Metallische Halbzeuge

Fraunhofer ITWM Fraunhofer IAIS Fraunhofer IWM

Overall workflow – How to find influential parameters for a given setting

- Look at regression plots to estimate the level of confidence for specific steel groups and fatigue ranges.
- Select relevant series
  - Bounding conditions
    - Steel Group
    - Steel Parameters
  - fatigue strength > minimum

  } relax selection criteria to get sufficient statistical support (nSeries > 100)
- Build ***several*** Decision Trees
  - look for interesting homogeneous subgroups
- Investigate interesting subsets
  - Plot histograms, refine decision tree, …
  - Compare with other subsets
- *repeat …*



ML-techniques used

- *scikit-learn* „Machine Learning in Python“
- Different models to choose from in ML-Tool:
  - RandomForestRegressor
    - „Random Forest shallow“: n_estimators = 10, max_depth = 5
    - „Random Forest deep“: n_estimators = 100, max_depth = 10
  - „Gradient Boosting Regressor“: n_estimators = 10, max_depth = 3
  - „ExtraTreesRegressor“: n_estimators = 100
  - „LinearRegression“
- **L**eave-**O**ne-**O**ut-**C**ross-**V**alidation LOOCV for model evaluation

Fatigue Database: Machine Learning

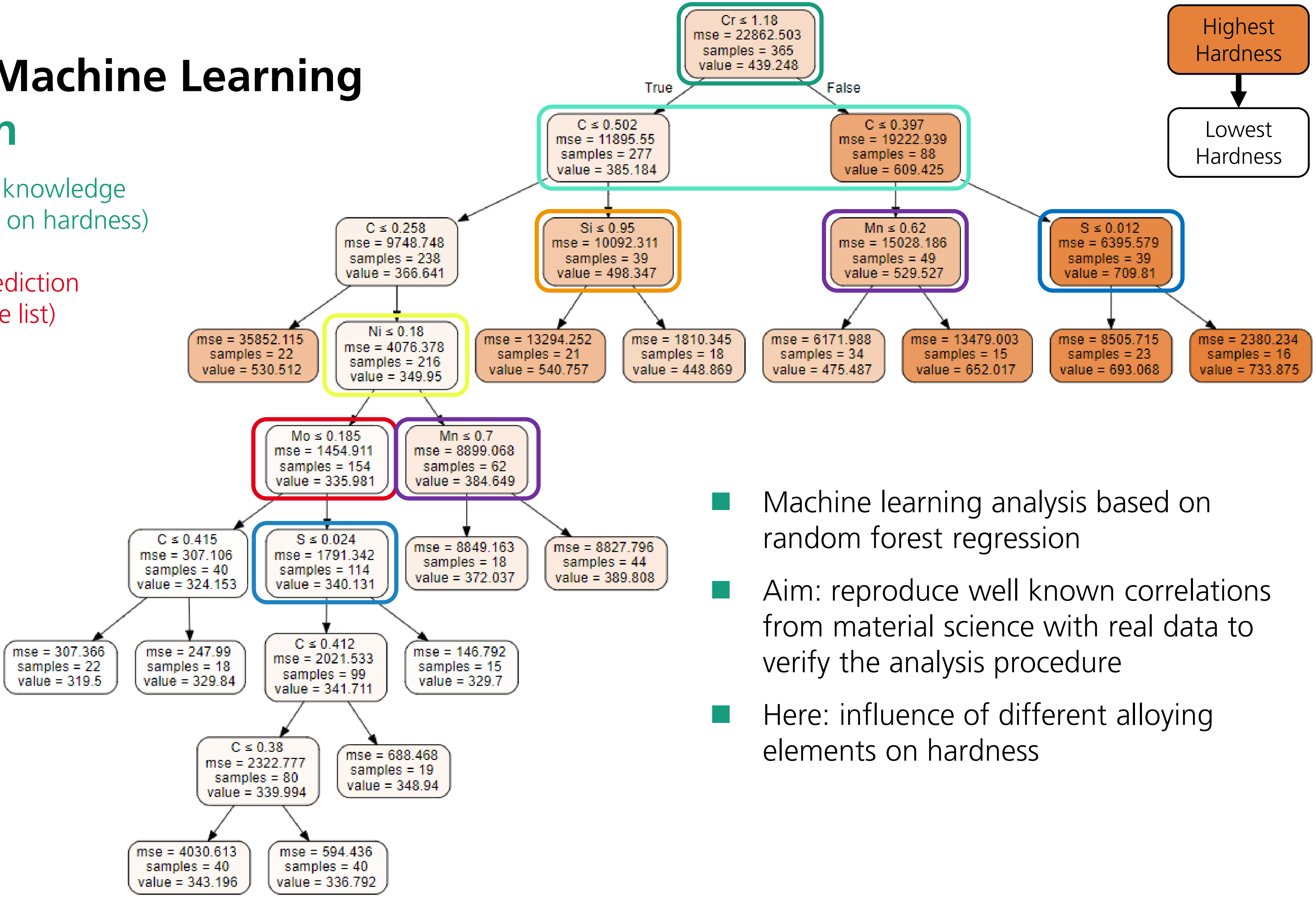
Hardness prediction

Exisiting material science knowledge
(effect of alloying elements on hardness)
vs.
Machine learning prediction
(feature importance list)

Legierungs-element		Härte
Si		↑
Mn	In perlit. Stählen	↑
Mn	In austenit. Stählen	↓↓↓
Cr		↑↑
Ni	In perlit. Stählen	↑
Ni	In austenit. Stählen	↓↓
Al		–
W		↑
V		↑
Co		↑
Mo		↑
Cu		↑
S		–
P		↑

from [1]

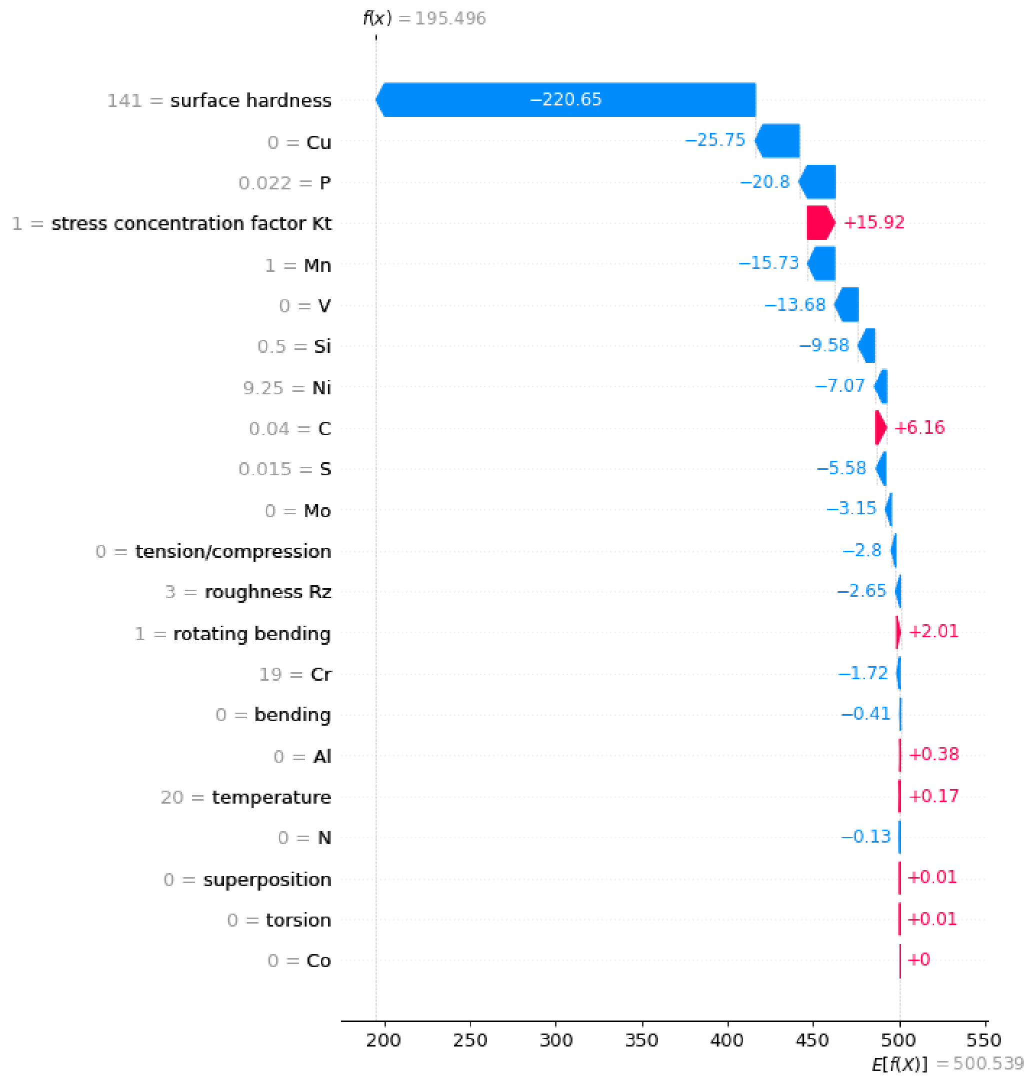
```
Cr: 0.471
C: 0.300
Ni: 0.066
Cu: 0.033
Si: 0.033
Mo: 0.031
Mn: 0.031
N: 0.023
S: 0.005
Al: 0.003
P: 0.003
V: 0.002
Co: 0.000
```



- Machine learning analysis based on random forest regression
- Aim: reproduce well known correlations from material science with real data to verify the analysis procedure
- Here: influence of different alloying elements on hardness

[1] Quelle: Vorlesung „Metallische Werkstoffe“, Ernst Fleischmann, Universität Bayreuth

Waterfall plot https://shap-lrjball.readthedocs.io/en/latest/example_notebooks/plots/waterfall.html



- Definition:
  - Waterfall plots are designed to display explanations for individual predictions, so they expect a single row of an Explanation object as input.
  - The bottom of a waterfall plot starts as the expected value of the model output, and then each row shows how the positive (red) or negative (blue) contribution of each feature moves the value from the expected model output over the background dataset to the model output for this prediction.
- Example:
  - Plot for first image of test dataset
  - Low surface hardness value leads to low predicted alternating strength
  - Kt=1 raises estimation by 16 MPa