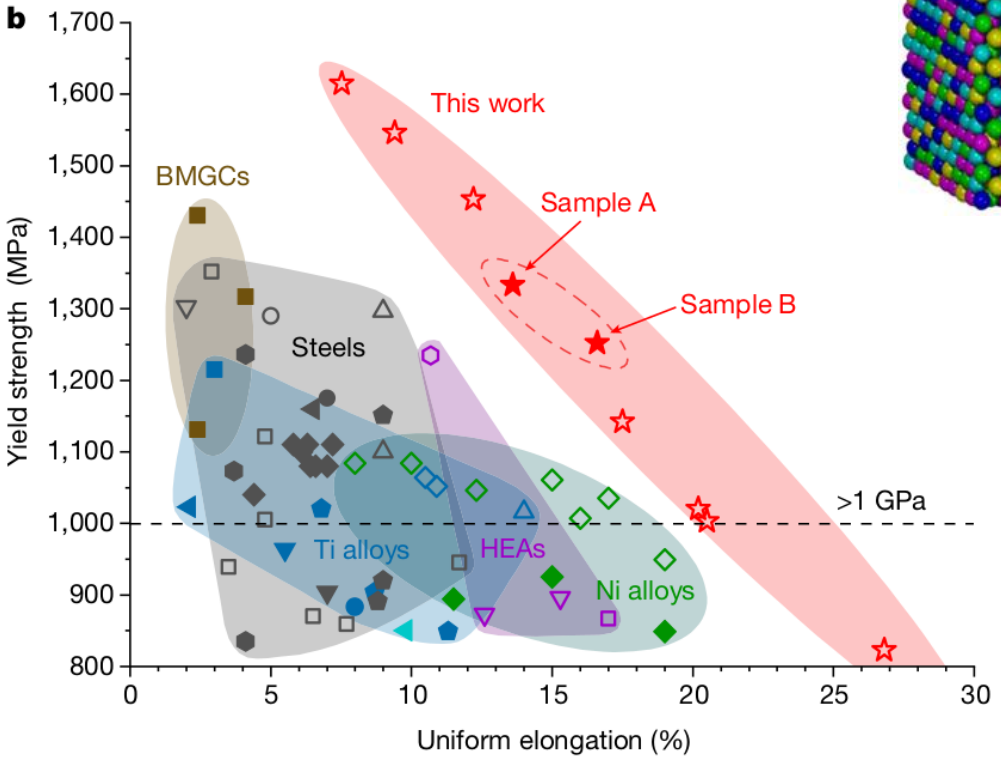
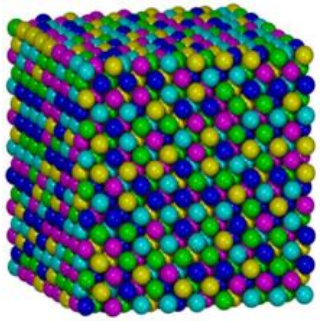
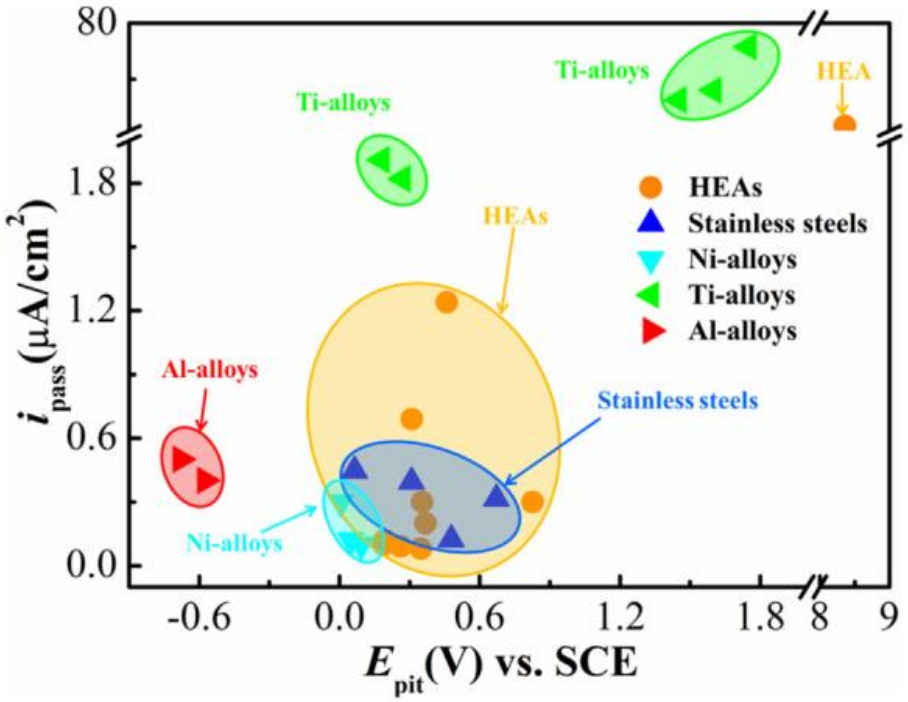
High-entropy alloys (HEAs)

Superior mechanical property





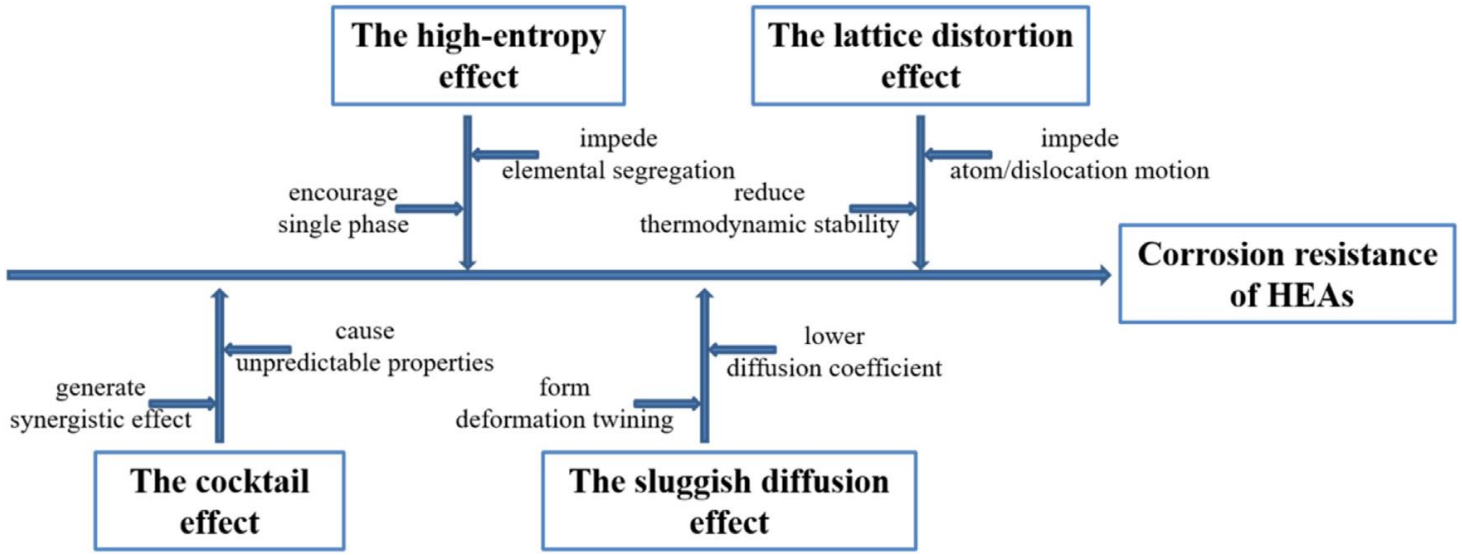
Superior localized corrosion resistance



Ren, J., Zhang, Y., Zhao, D. *et al*, ***Nature***, 608, 62–68 (2022)

Fu, Y. *et al*, ***J. Mater. Sci. Technol.***, 80, 217–233 (2021)

Core effects for high corrosion resistance of HEAs



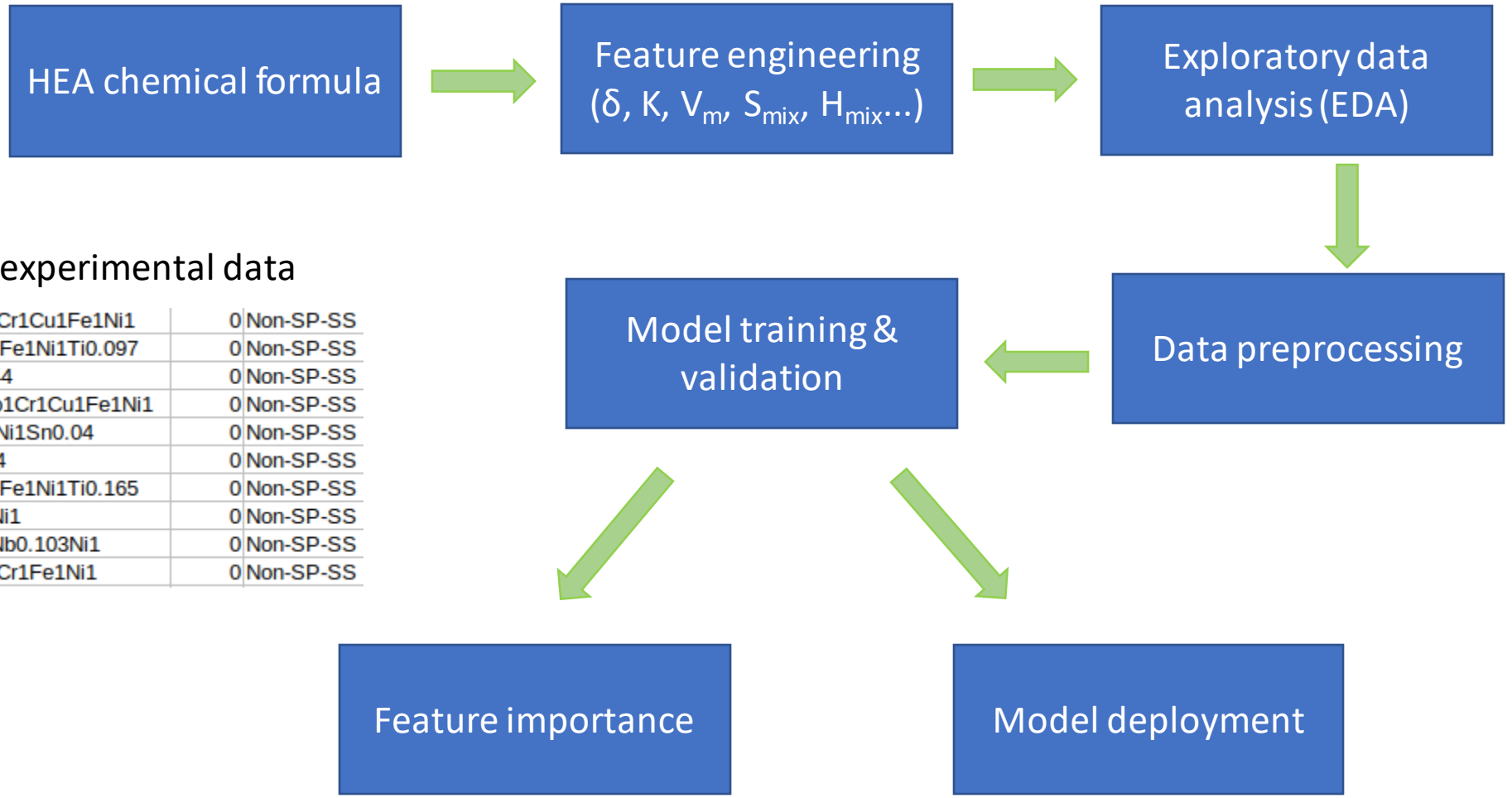
Fu, Y. *et al*, ***J. Mater. Sci. Technol.***, 80, 217–233 (2021)

Advantages of single-phase HEA

- Increased passivity
- Increased pitting resistance
- Reduced galvanic corrosion

Goal: Given the chemical formula, what is the probability of forming single-phase HEA?

Workflow of machine learning single-phase formability



Public experimental data

Al0.5B1Co1Cr1Cu1Fe1Ni1	0	Non-SP-SS
Co1Cu0.097Fe1Ni1Ti0.097	0	Non-SP-SS
Co0.56Cr0.44	0	Non-SP-SS
Al0.5B0.6Co1Cr1Cu1Fe1Ni1	0	Non-SP-SS
Co1Cu1Fe1Ni1Sn0.04	0	Non-SP-SS
Cr0.56Ni0.44	0	Non-SP-SS
Co1Cu0.165Fe1Ni1Ti0.165	0	Non-SP-SS
Co1Cr2Fe1Ni1	0	Non-SP-SS
Co1Cr1Fe1Nb0.103Ni1	0	Non-SP-SS
Al1C1.5Co1Cr1Fe1Ni1	0	Non-SP-SS

Data source: Yan, Y. et al., ***Computational Materials Science***, *199*, 2021.

Feature engineering

Description of the features.

Symbol	Description of Feature
δ	Atomic Size Difference
ΔH_{mix}	Mixing Enthalpy
ΔS_{mix}	Mixing Entropy
$\Delta\chi$	Pauli Electronegativity Difference
V_m	Molar Volume
K	Bulk Modulus
T_m	Melting Temperature
VEC	Valence Electron Concentration

Weighted average of atomic attributes

$$\Delta H_{mix} = 4 \sum_{i=1, i<j}^{n} H_{ij} c_i c_{ij},$$

$$\Delta\chi = \sqrt{\sum_{i=1}^{n} c_i (\chi_i - \bar{\chi})^2},$$

$$\Delta S_{mix} = -R \sum_{i=1}^{n} c_i \ln(c_i)$$

$$\delta = 100 \times \sqrt{\sum_{i=1}^{n} c_i (1 - \frac{r_i}{\bar{r}})^2},$$

Data sources

- Atomic sizes, melting temperature, valence electron concentration and molar volume are obtained from the mendeleev python package.
- Bulk modulus of each metal is excerpted from the plot on periodic table using WebPlotDigitizer.
- The pair mixing enthalpy is calculated based on Miedema model using code from qmpy python package.

Feature engineering

Raw data, 1807 entries

Al0.5B1Co1Cr1Cu1Fe1Ni1	0	Non-SP-SS
Co1Cu0.097Fe1Ni1Ti0.097	0	Non-SP-SS
Co0.56Cr0.44	0	Non-SP-SS
Al0.5B0.6Co1Cr1Cu1Fe1Ni1	0	Non-SP-SS
Co1Cu1Fe1Ni1Sn0.04	0	Non-SP-SS
Cr0.56Ni0.44	0	Non-SP-SS
Co1Cu0.165Fe1Ni1Ti0.165	0	Non-SP-SS
Co1Cr2Fe1Ni1	0	Non-SP-SS
Co1Cr1Fe1Nb0.103Ni1	0	Non-SP-SS
Al1C1.5Co1Cr1Fe1Ni1	0	Non-SP-SS

Feature engineered data

	Alloys	Class	k	vm	tm	vac	delta_s_mix	delta_chi	delta	delta_h_mix
1128	CoCrFeNiTi0.3	1	167.372093	7.165116	1876.870930	7.953488	12.825281	0.117413	1.811454	-13.527312
1429	Mo0.4Rh0.6	1	320.000000	8.740000	2499.750000	7.800000	5.595417	0.058788	3.524446	-21.504000
411	Al1Co1Cr1Fe1Mo1Ni0.67	0	164.714286	7.910406	1895.225838	6.825397	14.819798	0.184330	4.680815	-24.502736
533	Al1Co1Cr1Cu1Fe1Si1Ti1	0	133.142857	8.690000	1668.712857	6.428571	16.178290	0.141118	7.795787	-39.812245
1714	Al0.3HfNbTaTiZr	1	132.415094	11.886792	2433.356792	9.603774	14.431903	0.120383	5.376606	-9.693129

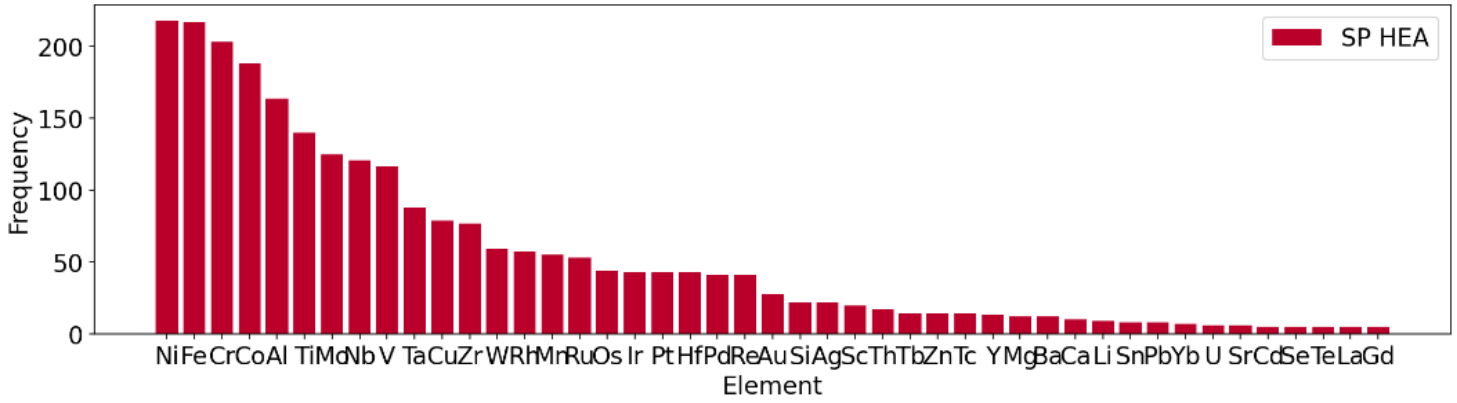
Exploratory data analysis

Balance of the dataset

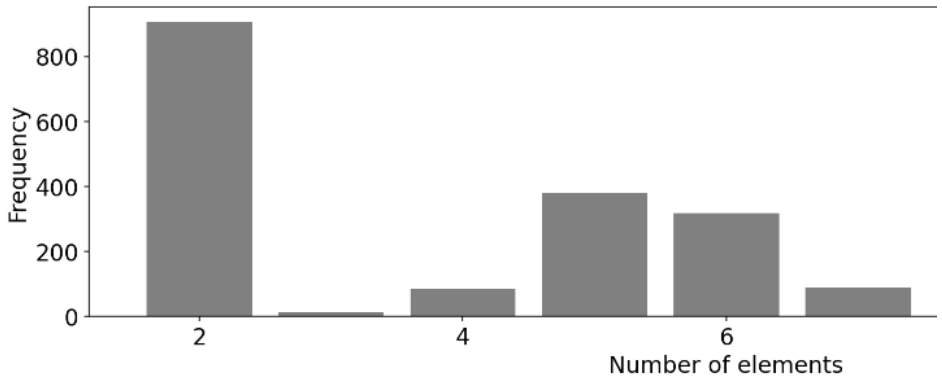
```
1  df['Class'].value_counts()/df['Class'].shape[0]
```

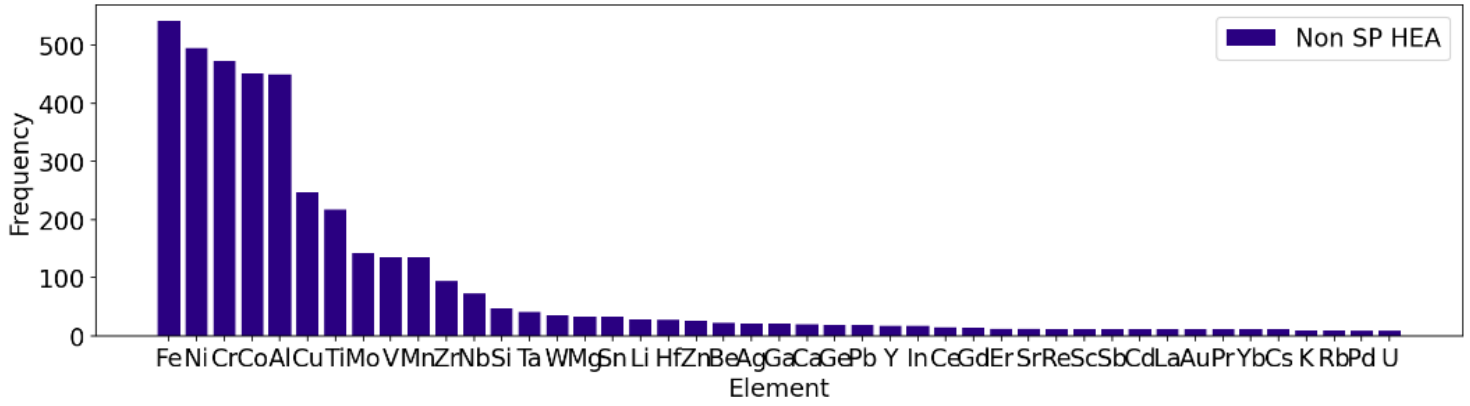
```
0    0.55285
1    0.44715
Name: Class, dtype: float64
```

Frequency of elements

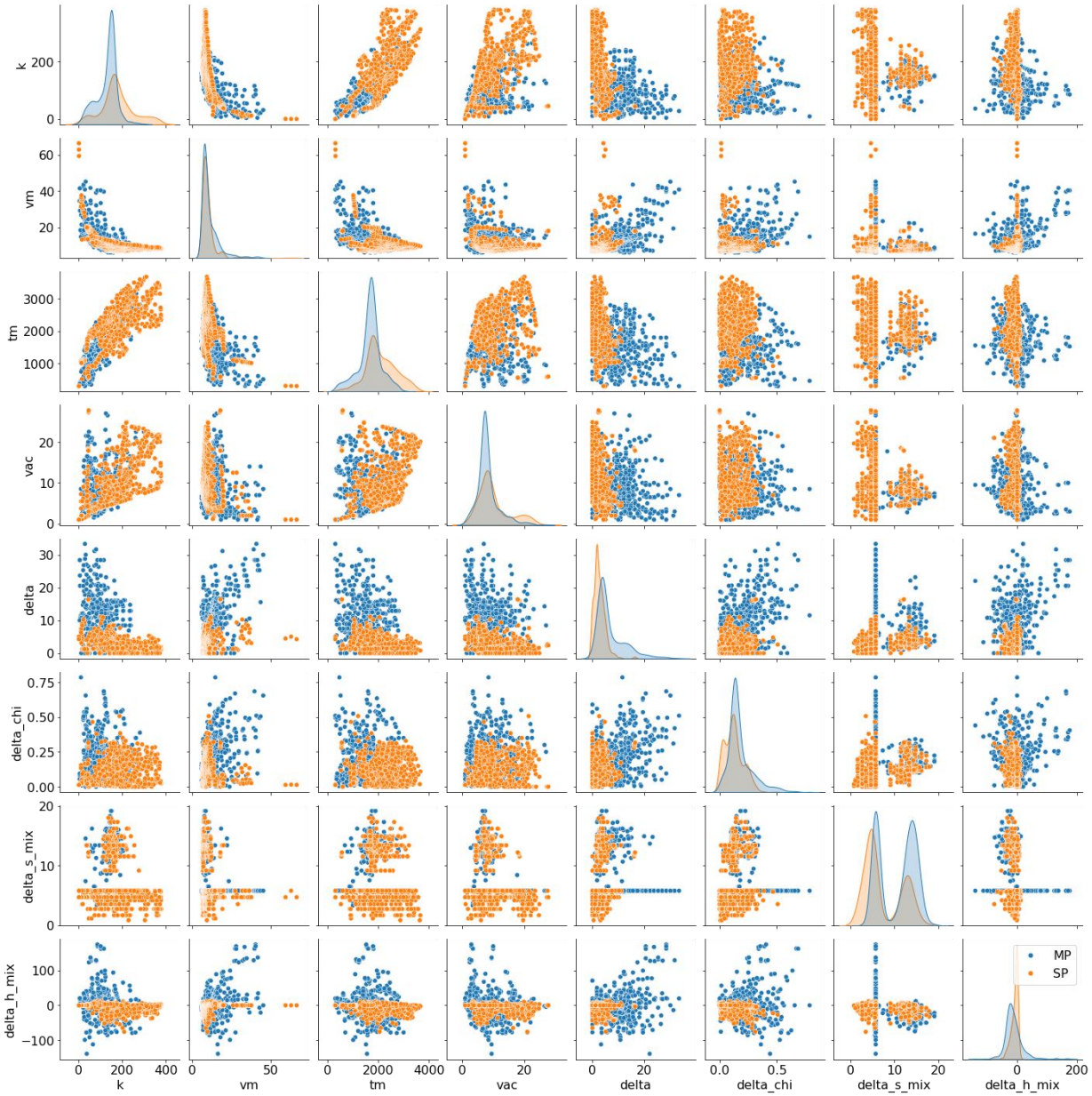


Frequency of # elements

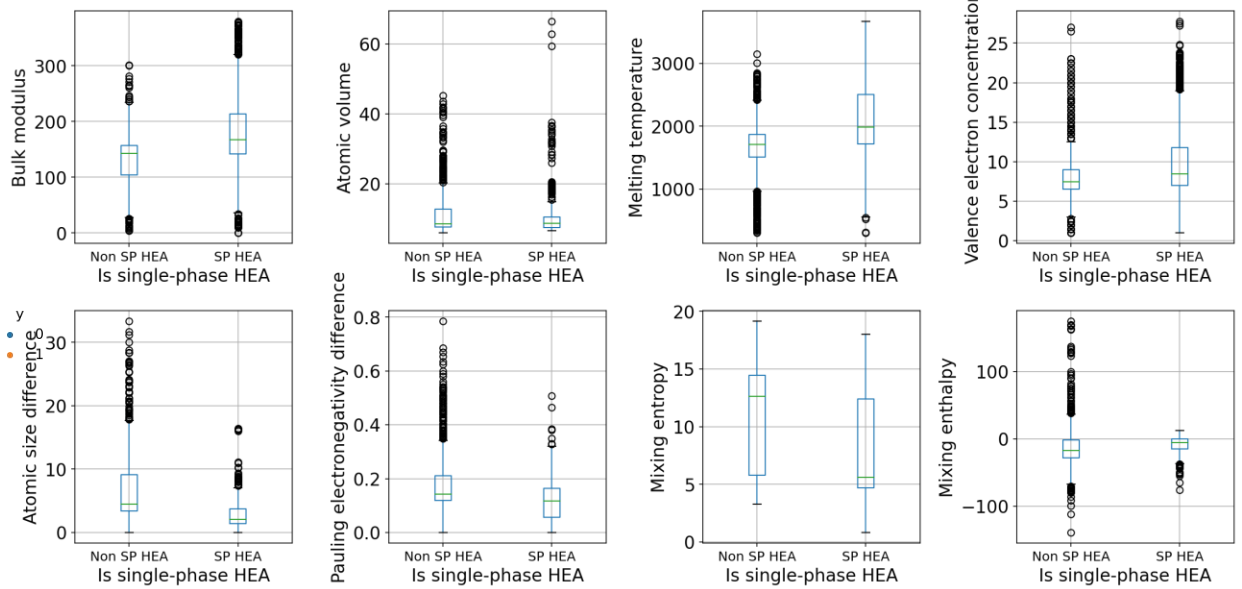




Feature-feature pair plot



Class-specific distribution of feature values



Data preprocessing

Minmax scaling for each numerical feature so that every feature has value in the range of [0, 1]

	Alloys	k	vm	tm	vac	delta	delta_chi	delta_s_mix	delta_h_mix
876	Er1Hf1	0.195884	0.165081	0.550199	0.560748	0.181818	0.038217	0.269946	0.487758
281	Al0.5Cr1Fe1Ni1V1	0.412654	0.026429	0.462762	0.215992	0.100974	0.151854	0.672726	0.362001
560	Co1Fe1Mn1Ti1V2.6Zr1	0.374031	0.047552	0.490520	0.183965	0.138086	0.210210	0.727235	0.373278
628	Pd40Cu30Ni10P20	0.353647	0.061699	0.334543	0.310280	0.349979	0.183674	0.536081	0.287135
758	Li1Si1	0.141802	0.108841	0.228212	0.056075	0.411765	0.585987	0.269946	0.383784

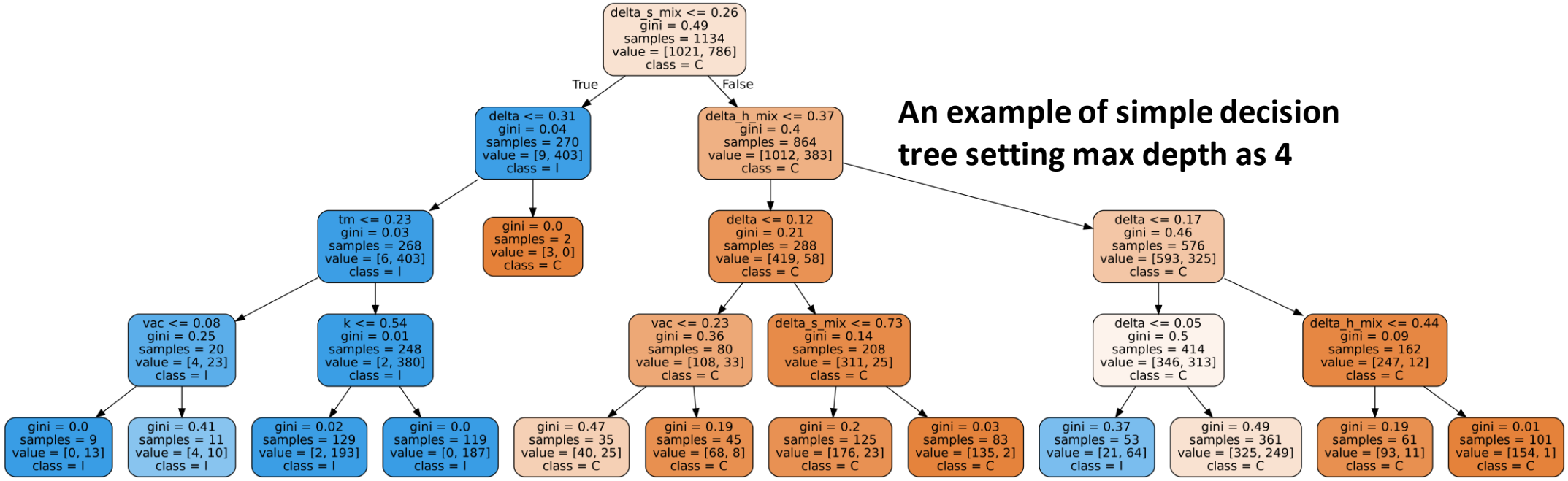
Model training

Three classification models and their accuracy scores

Methods	Accuracy score/stdev
Logistic regression	0.785/0.014
Neural network	0.785/0.015
Random Forest	**0.887/0.011**

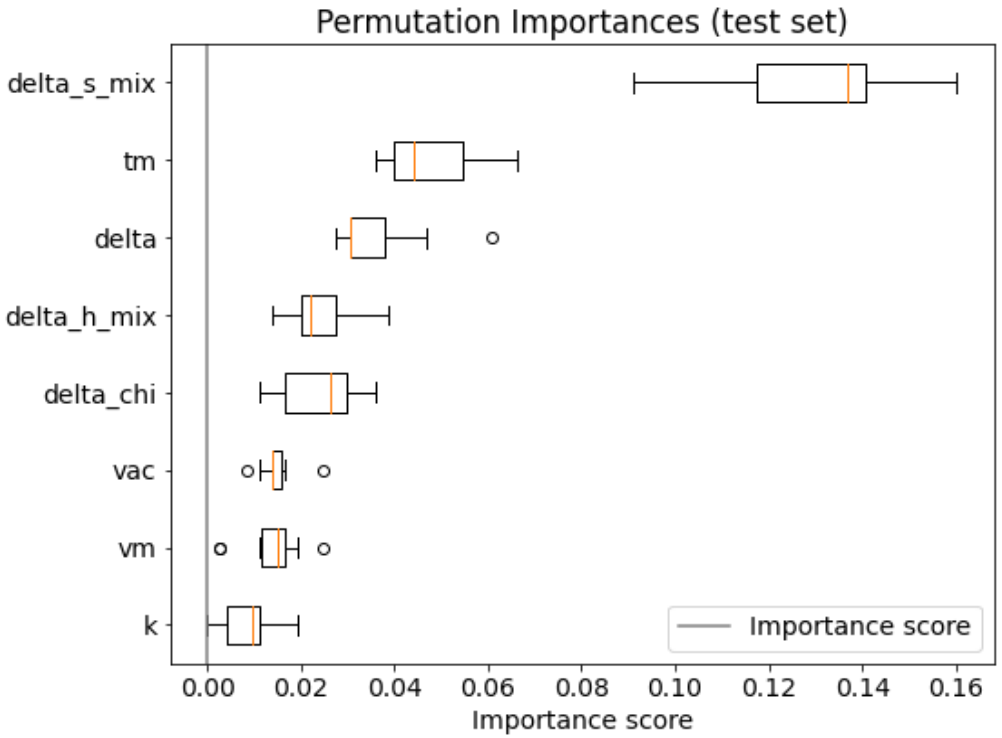
Best random forest model:

- **100 decision trees**
- **20 max depth**

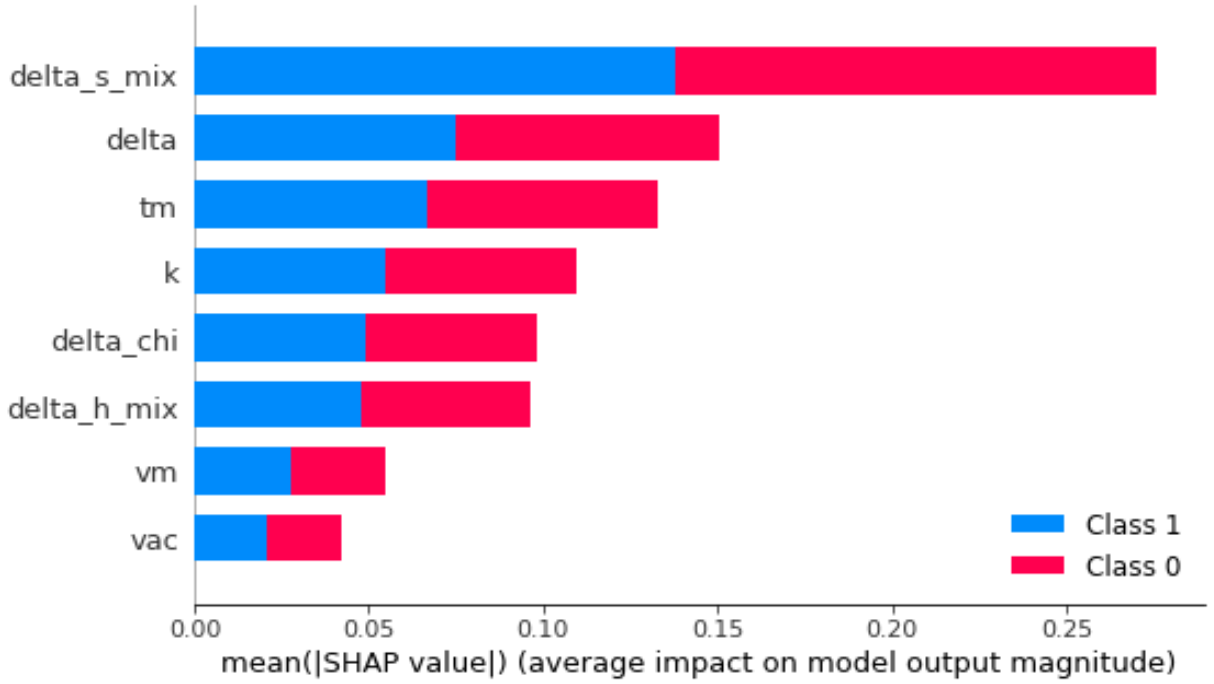


An example of simple decision tree setting max depth as 4

Feature importance



SHAP feature importance



Model deployment

['Ni', 'Fe', 'Cr', 'Co', 'Al', 'Ti', 'Mo', 'Cu']

Equimolar HEA alloys with five elements

```
NiFeCrCoAl : single phase.
NiFeCrCoTi : single phase.
NiFeCrCoMo : multiple phase.
NiFeCrCoCu : single phase.
NiFeCrAlTi : multiple phase.
NiFeCrAlMo : multiple phase.
NiFeCrAlCu : multiple phase.
NiFeCrTiMo : multiple phase.
NiFeCrTiCu : multiple phase.
NiFeCrMoCu : single phase.
NiFeCoAlTi : multiple phase.
NiFeCoAlMo : multiple phase.
NiFeCoAlCu : multiple phase.
NiFeCoTiMo : multiple phase.
NiFeCoTiCu : multiple phase.
NiFeCoMoCu : single phase.
NiFeAlTiMo : multiple phase.
NiFeAlTiCu : multiple phase.
NiFeAlMoCu : multiple phase.
NiFeTiMoCu : multiple phase.
NiCrCoAlTi : multiple phase.
NiCrCoAlMo : multiple phase.
NiCrCoAlCu : multiple phase.
NiCrCoTiMo : multiple phase.
NiCrCoTiCu : multiple phase.
NiCrCoMoCu : single phase.
```

['Ni', 'Fe', 'Cr', 'Co', 'Mo']

Fixed element types, varied compositions

	Alloy	Co	Cr	Ni	Mo	class_pred
490	Co20Cr15Ni17Mo10Fe38	20	15	17	10	1
869	Co18Cr16Ni18Mo14Fe34	18	16	18	14	0
3067	Co19Cr20Ni15Mo7Fe39	19	20	15	7	1
2108	Co20Cr18Ni17Mo8Fe37	20	18	17	8	1
1014	Co20Cr16Ni16Mo9Fe39	20	16	16	9	1
407	Co19Cr15Ni18Mo2Fe46	19	15	18	2	1
934	Co19Cr16Ni17Mo4Fe44	19	16	17	4	1
990	Co20Cr16Ni15Mo0Fe49	20	16	15	0	1
540	Co15Cr16Ni15Mo0Fe54	15	16	15	0	1
1053	Co20Cr16Ni19Mo3Fe42	20	16	19	3	1
2555	Co19Cr19Ni17Mo5Fe40	19	19	17	5	1
339	Co18Cr15Ni19Mo9Fe39	18	15	19	9	1
547	Co15Cr16Ni15Mo7Fe47	15	16	15	7	1
3234	Co20Cr20Ni20Mo9Fe31	20	20	20	9	1
345	Co18Cr15Ni20Mo0Fe47	18	15	20	0	1
2674	Co20Cr19Ni19Mo4Fe38	20	19	19	4	1
963	Co19Cr16Ni19Mo3Fe43	19	16	19	3	1
597	Co15Cr16Ni18Mo12Fe39	15	16	18	12	0
347	Co18Cr15Ni20Mo2Fe45	18	15	20	2	1
134	Co16Cr15Ni17Mo14Fe38	16	15	17	14	0