Artificial intelligence for material selection

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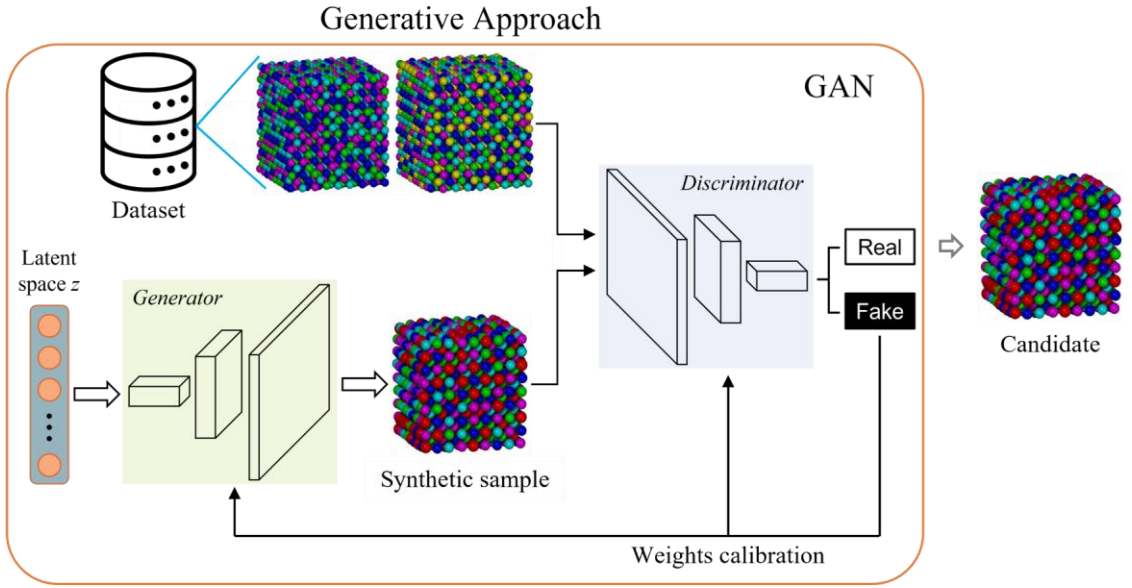
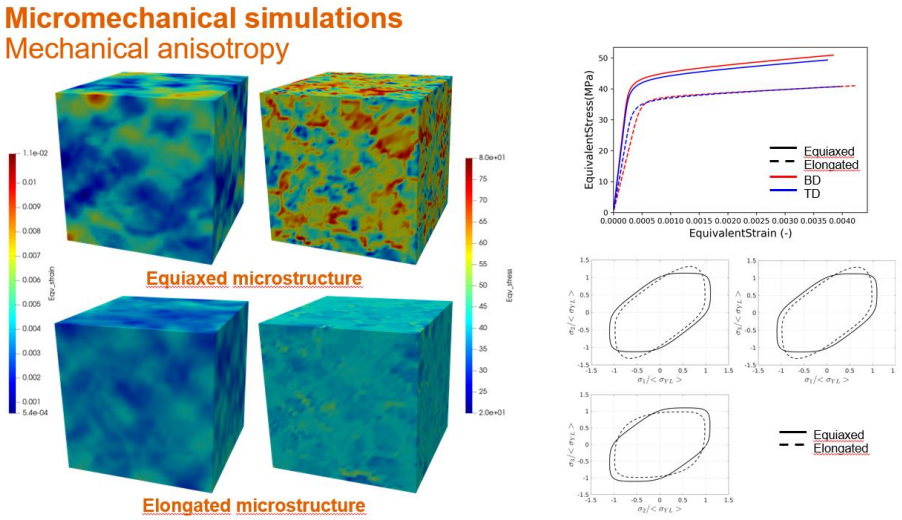
VTT

The project has received funding from the European Union's Horizon 2020 research and innovation program under Grant Agreement N° 958374.

Content

- Use case
- HEA/CCA
- Alloy design approach
- Design workflow
- Steps after the alloy design





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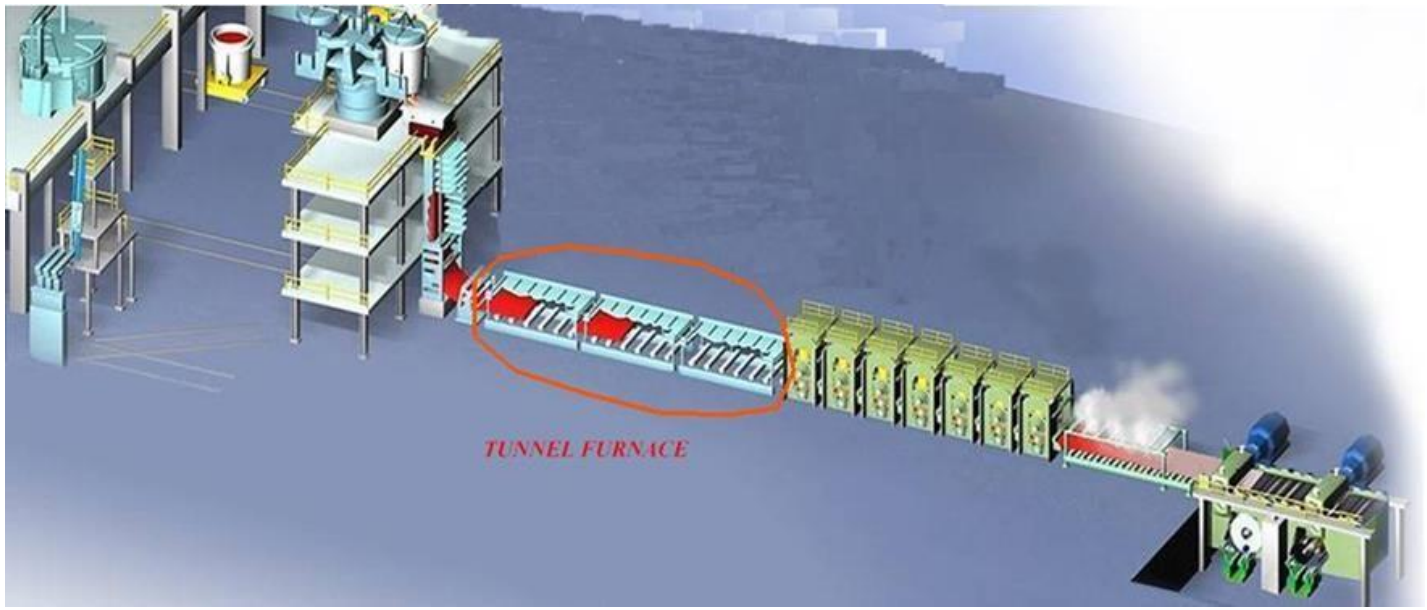
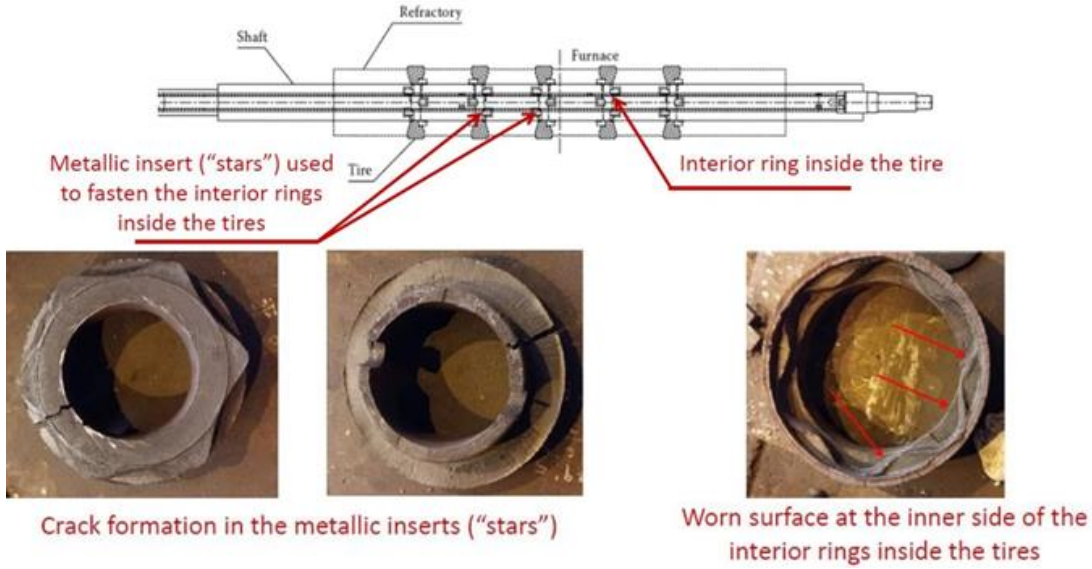
Use case for AI designed alloy

Inserts (stars) (ARCELOR MITTAL)

→ Main goal : to decrease repair damaged and cooled water consumption by improving high temperature strength and creep resistance in tunnel furnace





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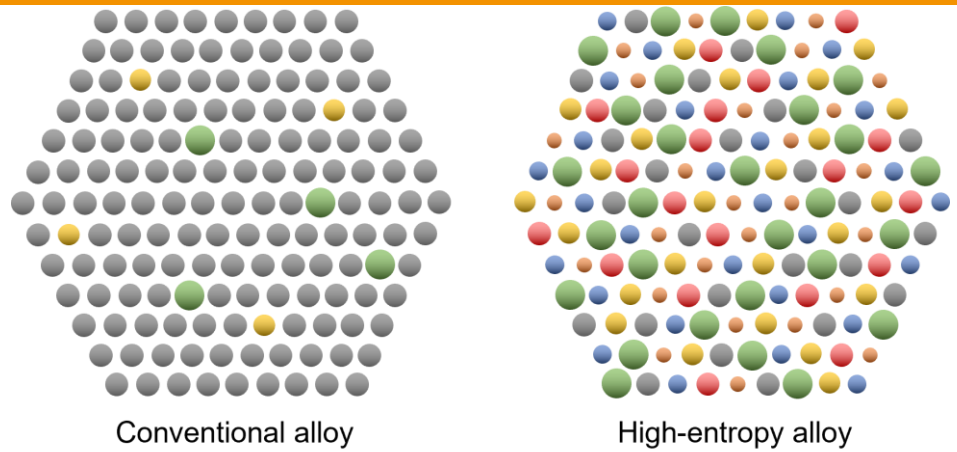
High Entropy Alloys (HEAs)/ Complex Consentrated Alloys (CCA)

Class of materials containing more than 4-5 principal elements that have a mixture of simple FCC, BCC, and HCP structures.

- They can appear in different phases : solid solution (SS), intermetallic (IM), amorphous (AM), or a mix of them.



Many HEAs have higher strength than traditional alloys even in elevated temperatures

- The BCC metals often have very high yield strengths with limited ductility.
- The FCC metals have high ductility but low strength

→ The mixture of BCC + FCC is expected to possess balanced mechanical properties.

Based on high entropy concept

$$\Delta S = -R \sum_{i=1}^{n} c_i \ln c_i$$

$$\Delta G = \Delta H - T\Delta S$$

n	1	2	3	4	5	6	7	8	9	10	11	12	13
ΔS_{conf}	0	0.69R	1.1R	1.39R	1.61R	1.79R	1.95R	2.08R	2.2R	2.3R	2.4R	2.49R	2.57R

low | medium | high entropy →

1.0R 1.5R

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Challenges in HEA/CCA design

Hit and trial method

- No phase diagram
- Does not follow traditional (emperical) rules
- Huge number of combinations

Ab initio simulation

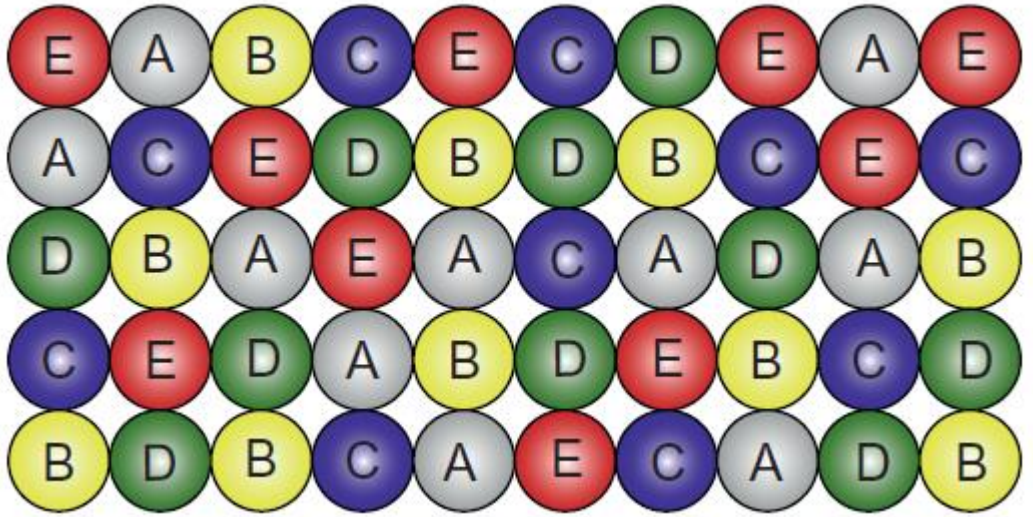
- Availability of suitable potentials?
- Huge computing power and time required

Parametric approach

- Relatively new material group
- Not enough scientific background

CALPHAD

- Limited reliable databases
- Time and cost effective



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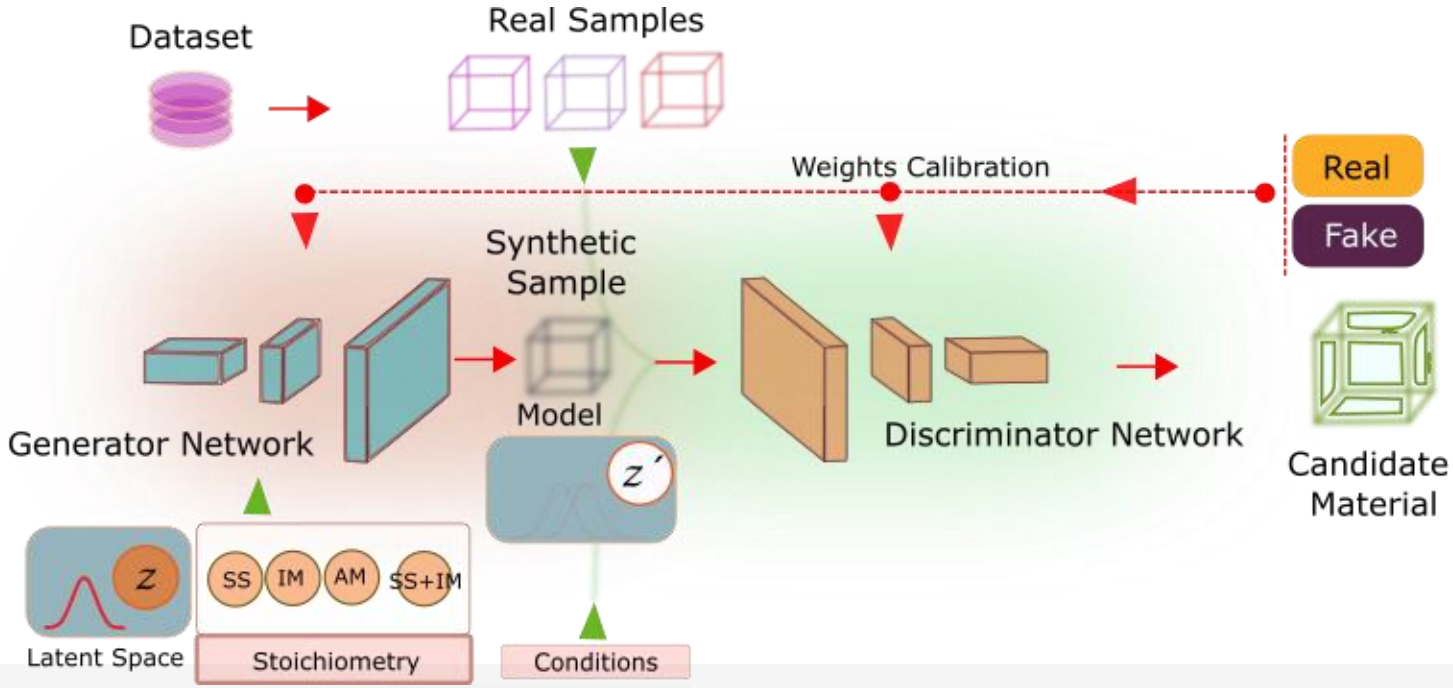
Workflow for generating new alloy candidates

- The used approach is based on Generative Adversarial Networks (GAN).
- Datasets have been developed, containing data from real samples, and used as a training data.
- After trained, the model can generate synthetic samples, based on the features (design parameters) learned from the real samples.



1. Developed dataset
2. Train neural Network with the dataset
3. Generate synthetic candidates
4. Validate candidates

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High entropy alloys design parameters:

Based on literature a dataset was created.

1. 15 features (in the table)
2. Number of elements
3. Phase (amorphous, intermetallic, solid solution, and a mix of intermetallic + solid solution)
4. 78 chemical elements with their corresponding concentration

Features	Equations
Mean atomic radius	$a = \sum_i c_i \cdot r_i$
Atomic size difference	$\delta = \sqrt{\sum_i \left(c_i \cdot \left(1 - \frac{r_i}{\sum_i c_i \cdot r_i} \right)^2 \right)}$
Average melting temperature	$T_m = \sum_i c_i \cdot T_{mi}$
Standard deviation of melting temperature	$\sigma_T = \sqrt{\sum_i c_i \cdot \left(1 - \frac{T_{mi}}{T_m} \right)^2}$
Mixing enthalpy	$\Delta H_{mix} = 4 \sum_{i \neq j} c_i \cdot c_j \cdot H_{ij}$
Standard deviation of mixing enthalpy	$\sigma_{\Delta H} = \sqrt{\sum_{i \neq j} c_i \cdot c_j \cdot (H_{ij} - \Delta H_{mix})^2}$
Mixing entropy	$\Delta S_{mix} = -R \sum_i c_i \cdot \log c_i$
Electronegativity	$\chi = \sum_i c_i \cdot \chi_i$
Standard deviation of electronegativity	$\Delta \chi = \sqrt{\sum_i \left(c_i (\chi_i - \chi)^2 \right)}$
Valence electron concentration	$VEC = \sum_i c_i \cdot VEC_i$
Standard deviation of VEC	$\sigma_{VEC} = \sqrt{\sum_i \left(c_i \cdot (VEC_i - VEC)^2 \right)}$
Mean bulk modulus	$K = \sum_i c_i \cdot K_i$
Standard deviation of bulk modulus	$\sigma_K = \sqrt{\sum_i c_i \cdot (K_i - K)^2}$
Young modulus	$E = \sum_i c_i E_i$
Shear modulus	$G = \sum_i c_i G_i$

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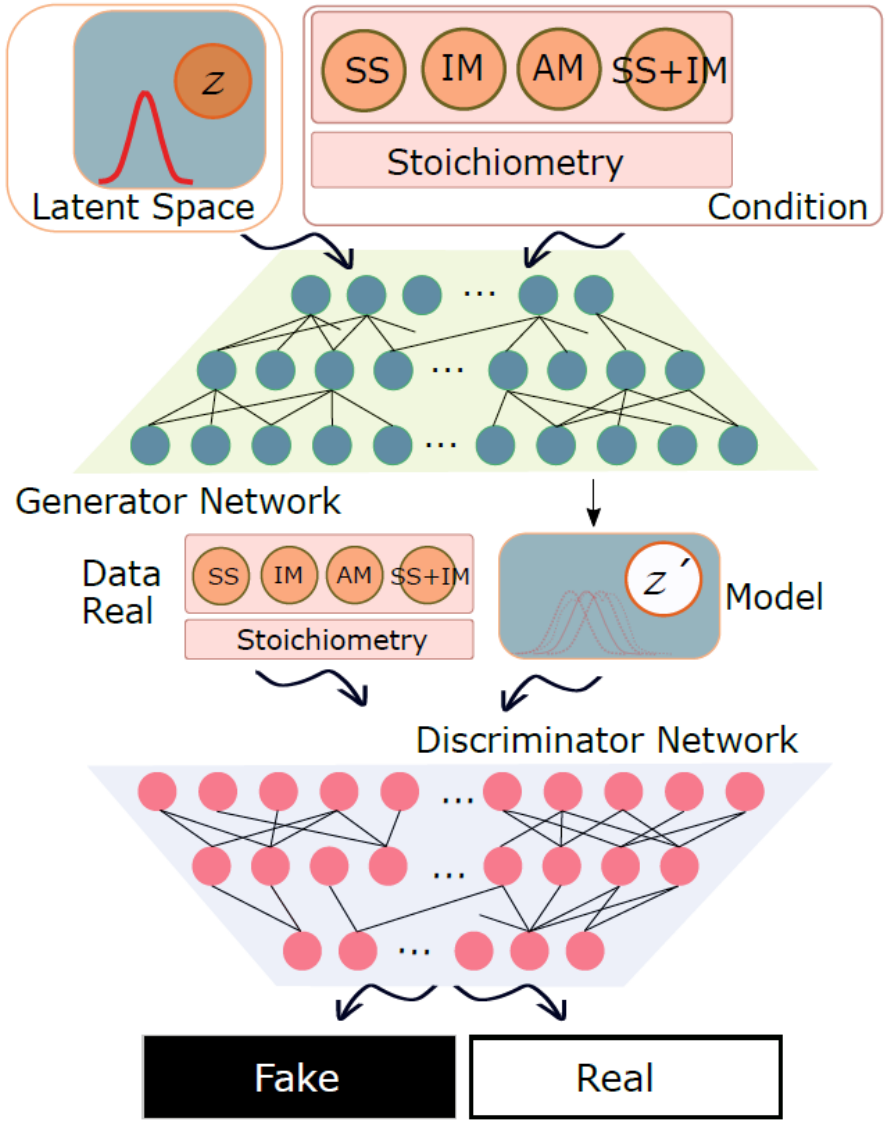
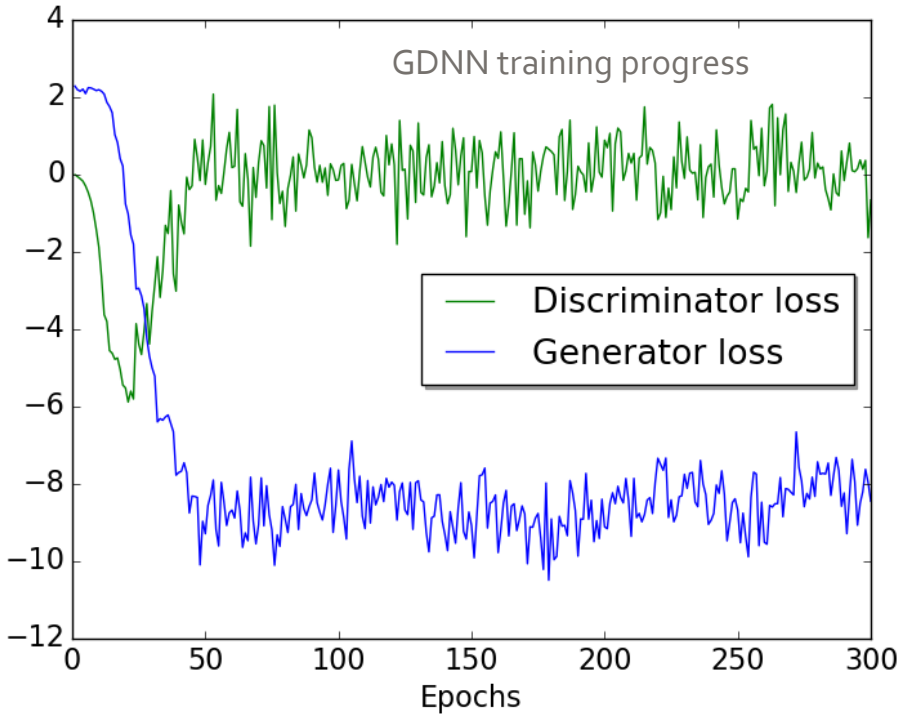
Training the model



	Generator		Discriminator	
Layer	Type	Dimension	Type	Dimension
Input	Latent + Cond.	90	Features + Cond	71
Hidden 1	Dense layer	256	Dense layer	256
Hidden 2	Dense layer	128	Dense layer	128
Output	Dense layer	71	Dense layer	1



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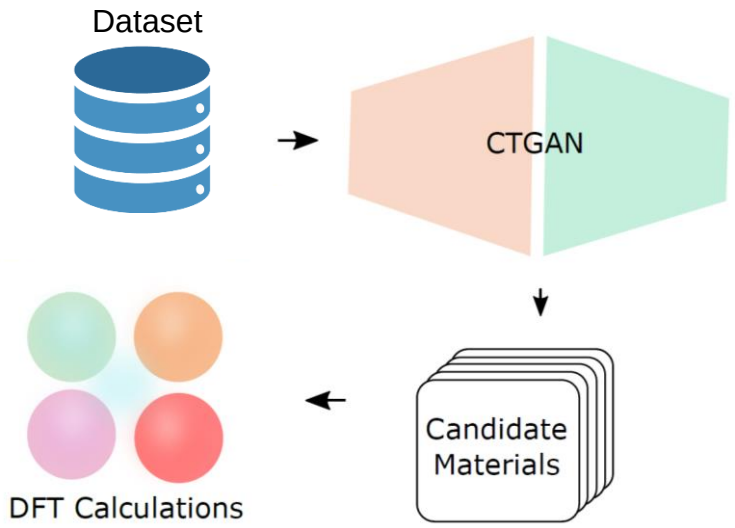
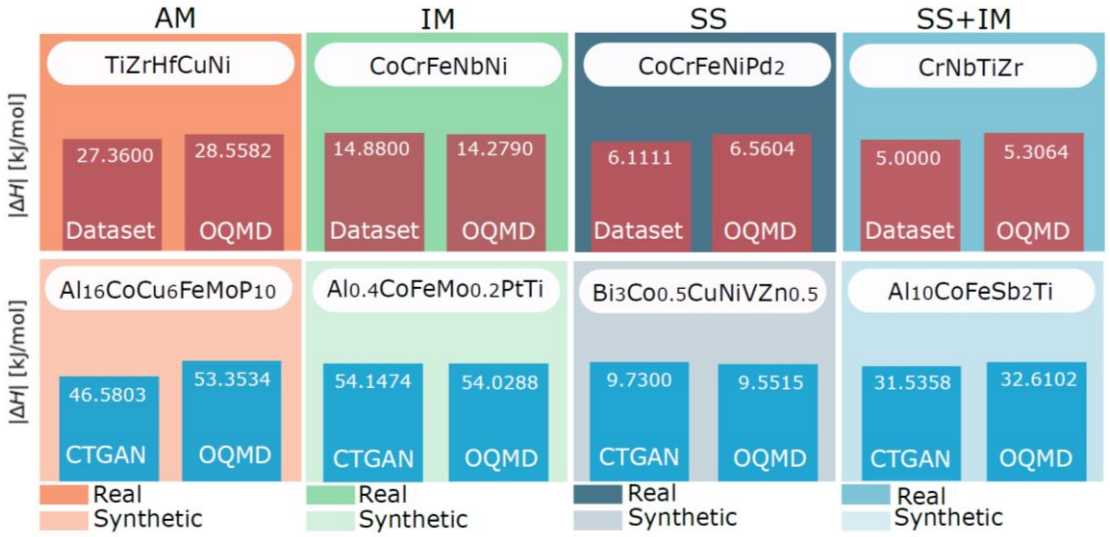
Validation of GAN

➢Validation methods

- Verification of generated samples which were not included at the training dataset
- Comparison between DFT-based calculation and NN enthalpy for HEA.





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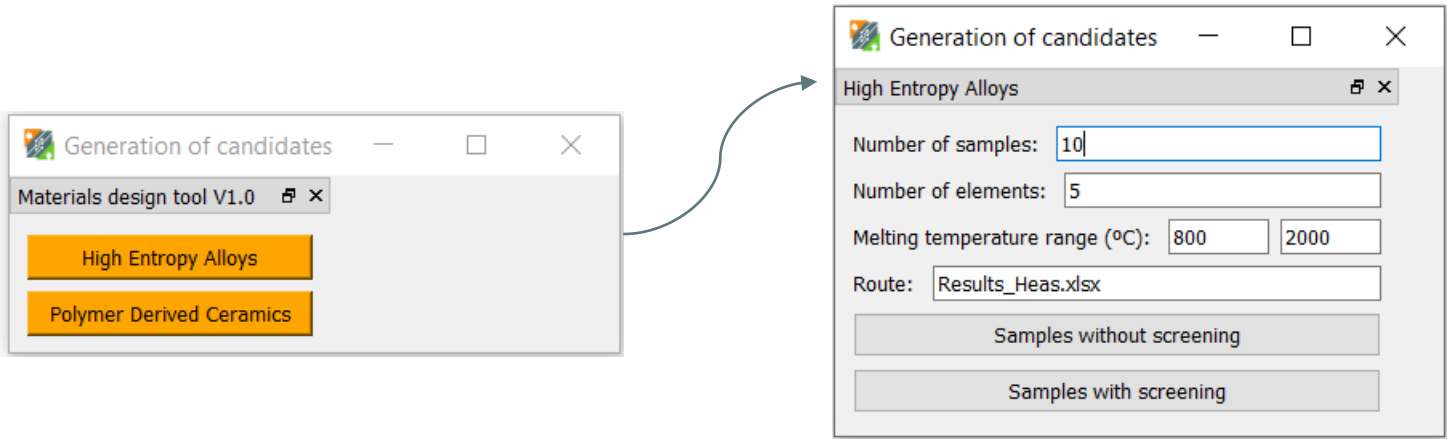
Materials Design Tool

Tool for generating high entropy alloys based on this methodology.



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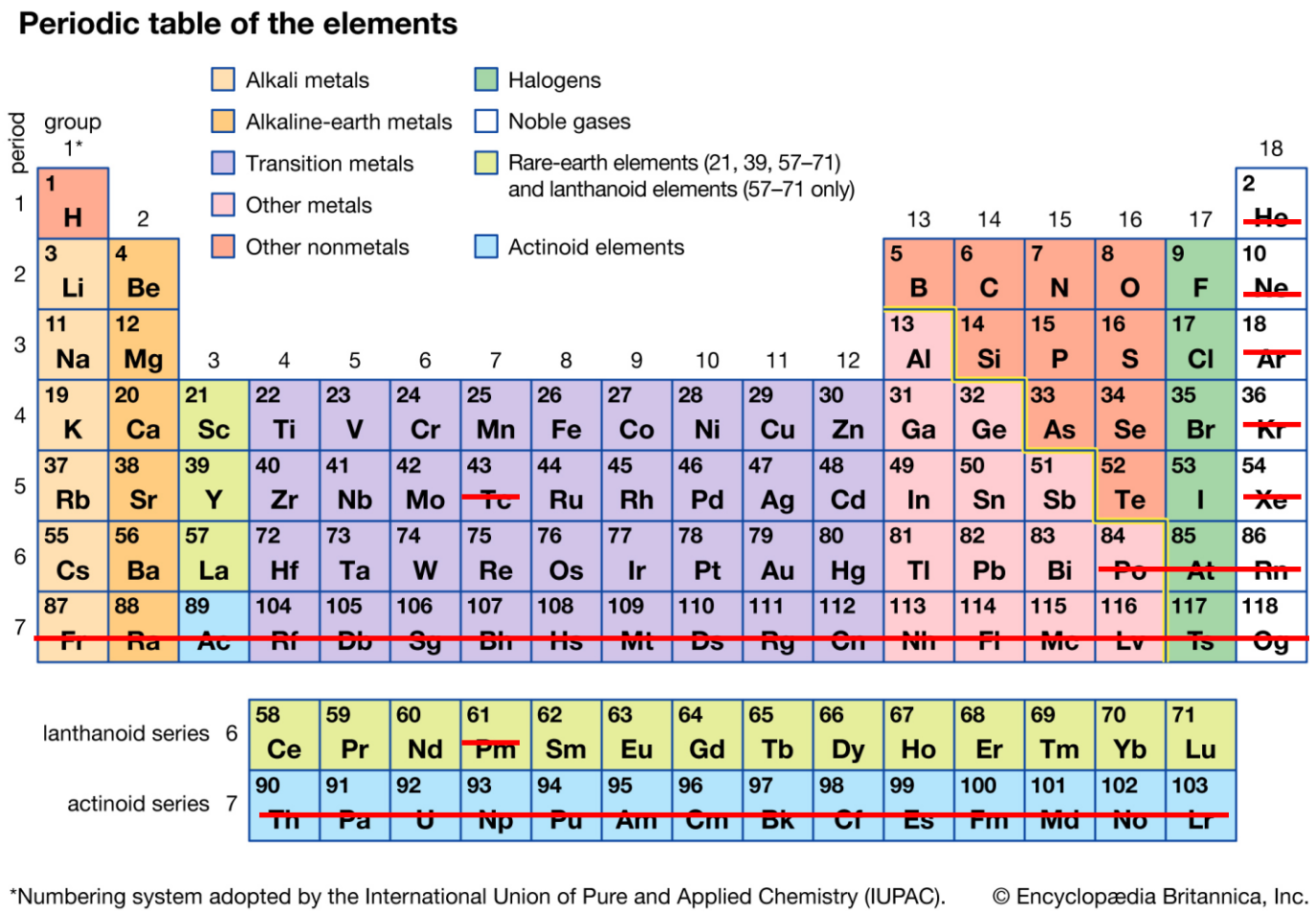
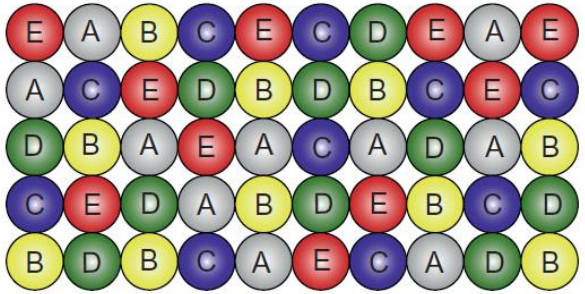
Screening for simulation



- **Initial approach:**
- Noble gases and radioactive elements removed
- A total of 78 chemical elements remained



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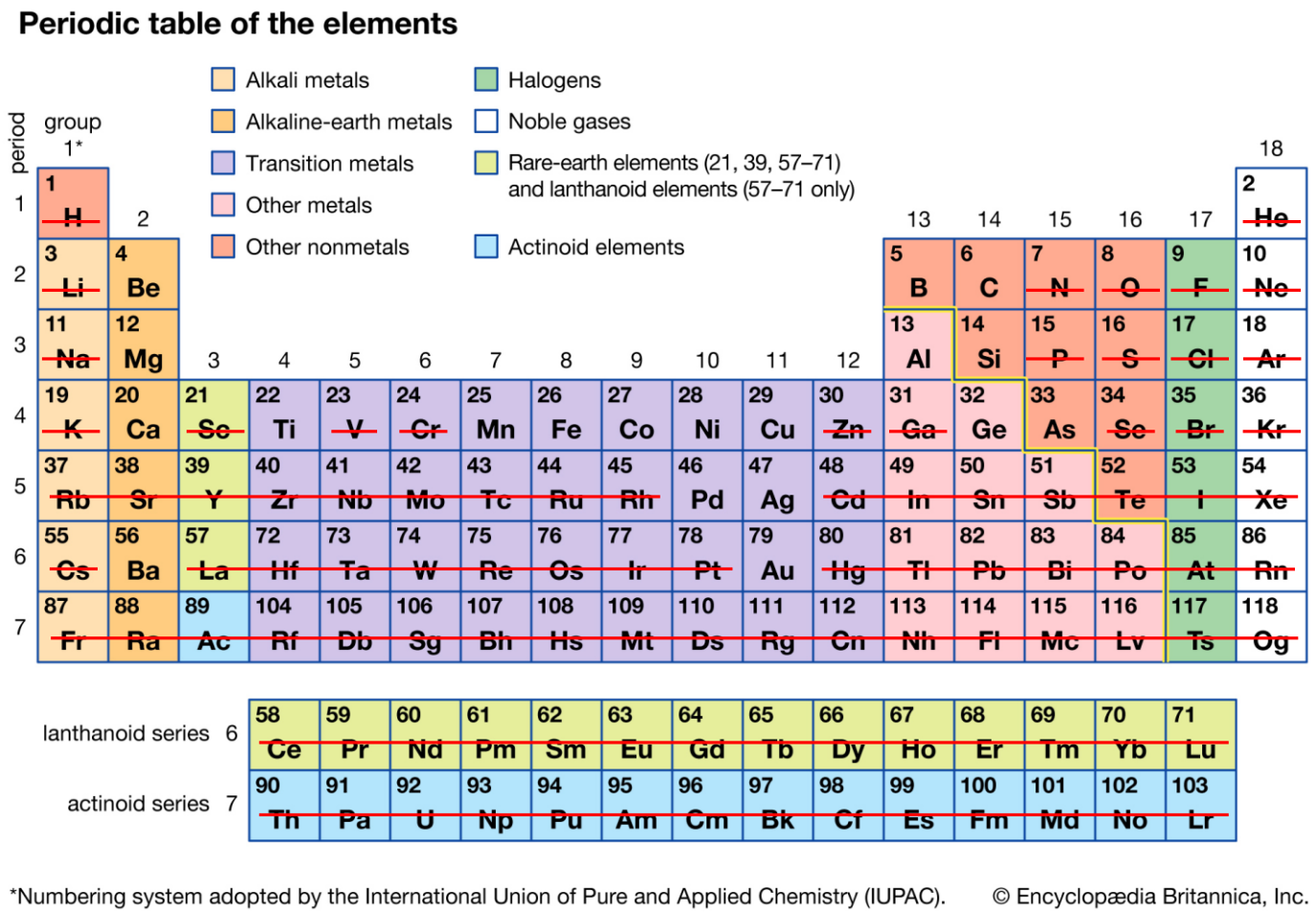
Screening for simulation



- Noble gases removed.
- Radioactive elements removed.
- Rare-earth elements removed.
- Toxic elements removed.
- Expensive elements removed.
- Elements with T_m > 2000 °C removed.
- A total of 19 chemical elements remained.

$$\binom{19}{5} = 11\,628 \qquad \binom{19}{6} = 27\,132$$

$$\binom{19}{7} = 50\,388 \qquad \binom{19}{8} = 75\,582$$

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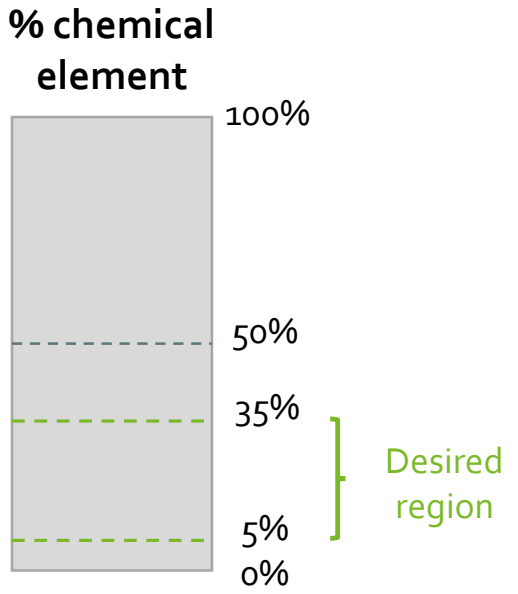
Screening for simulation

- Following prior experience on suitable materials for the use case, compounds that include Ni, Al and Si were promoted.

- No more than 35% per chemical element.



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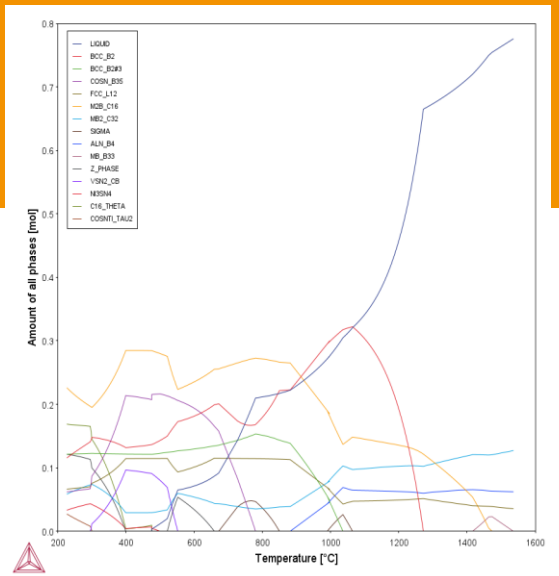
Evaluate GAN results

AlB2CoCr4.5FeMoNNiSn3TiV



- Only one new alloy will be produced
- Used TC (and prior experience) to evaluate the GAN results → some elements are not in relevant database (TCHEA4) thus alloys needed to be neglected or modified
- Fast screening of candidate by verifying the solidus/liquidus temperatures
- Phase equilibrium diagrams messy in many alloys → presence of wanted phases?

- B and C only as minor alloying elements
- Co expensive (and health issues)
- Exclude compositions with too low solidus and liquidus
- Neglect alloys with elements with too high liquidus -> not manufacturable with current means

Out[630]= {Al, B, C, Co, Cu, Fe, Mn, Ni, Si, Ti, T_liquidus, T_solidus}

Out[631]//MatrixForm=

{0.25, 0., 0., 0.25, 0., 0., 0., 0.25, 0., 0.25}	1812.72	1694.57
{0.25, 0., 0., 0., 0., 0.25, 0.25, 0., 0., 0.25}	1676.6	1602.61
{0.222222, 0., 0., 0.222222, 0., 0.222222, 0.222222, 0.111111, 0., 0.}	1776.91	1602.4
{0.25, 0., 0., 0.25, 0., 0., 0., 0.25, 0., 0.25}	1812.72	1694.57
{0.125, 0.375, 0., 0., 0., 0.1875, 0.1875, 0., 0., 0.125}	5398.68	1680.49
{0.0830565, 0., 0., 0.415282, 0.0332226, 0.468439, 0., 0., 0., 0.}	1692.77	1669.86
{0.0322581, 0.903226, 0., 0.0645161, 0., 0., 0., 0., 0., 0.}	2298.85	1625.04
{0.138889, 0., 0.0277778, 0., 0., 0.277778, 0.277778, 0., 0., 0.277778}	4824.59	1612.48
{0.25, 0., 0., 0.25, 0., 0.25, 0., 0.25, 0., 0.}	1779.37	1684.37
{0., 0., 0., 0.222222, 0.222222, 0.222222, 0., 0.333333, 0., 0.}	1664.51	1609.29
{0.222222, 0., 0., 0.222222, 0., 0.222222, 0., 0.333333, 0., 0.}	1733.83	1633.74
{0.25, 0., 0., 0.25, 0., 0.25, 0., 0.25, 0., 0.}	1779.37	1684.37
{0.243902, 0., 0., 0.243902, 0., 0.243902, 0., 0.243902, 0.0243902, 0.}	1770.58	1610.74
{0.25, 0., 0., 0.25, 0., 0.25, 0., 0.25, 0., 0.}	1779.37	1684.37
{0.25, 0., 0., 0.25, 0., 0.25, 0., 0.25, 0., 0.}	1779.37	1684.37
{0.25, 0., 0., 0.25, 0., 0., 0., 0.25, 0., 0.25}	1812.72	1694.57
{0.142857, 0., 0., 0.285714, 0., 0.285714, 0., 0.285714, 0., 0.}	1648.31	1637.36
{0.25, 0., 0., 0., 0., 0.25, 0.25, 0.25, 0., 0.}	1901.11	1610.97
{0.176471, , , , , 0.235294, 0.235294, 0.235294, 0.117647, }	2001.51	1654.5

(*note from above, there are some rather decent ones which comprise of cheap elements, i.e., Al, Fe,Mn; with Ni-Ti*)

At%

Nd	Ti	Al	Cu	Mo
22.2	22.2	22.2	22.2	11.1

no Nd in TCHEA4 →

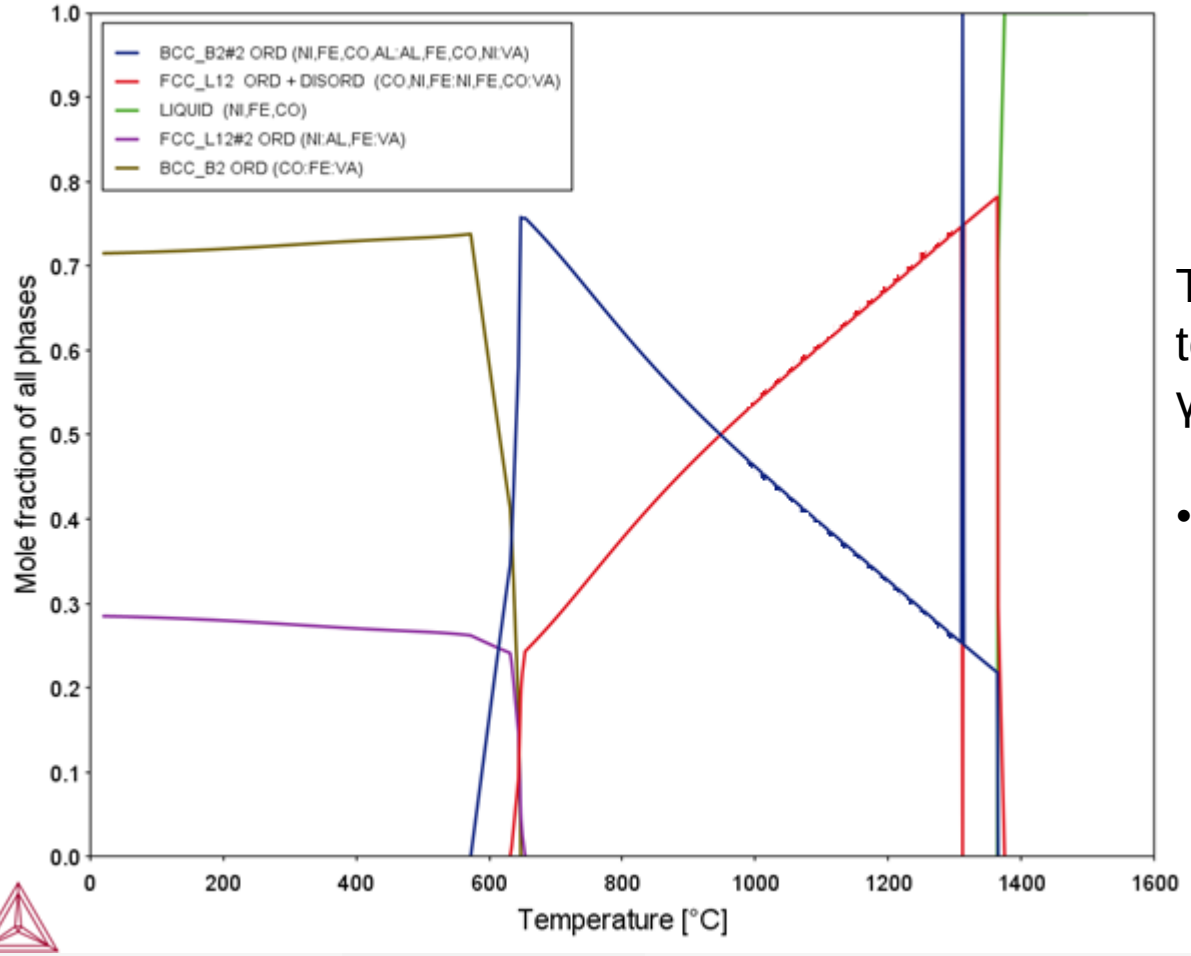
At%

Ti	Al	Cu	Mo
28.6	28.6	28.6	14.3

ACHIEF

The project has received f
research and innovation p

Candidate alloy

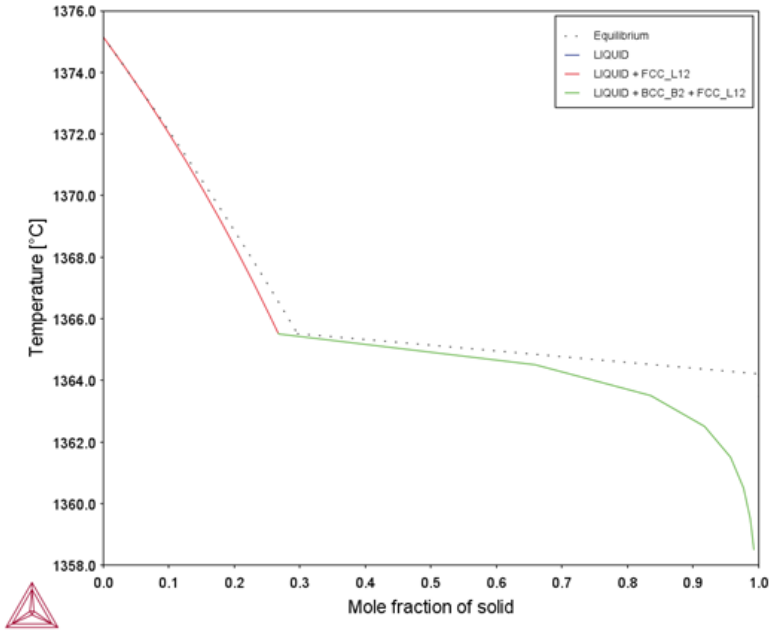


Component	*Mole Fraction*	*Mass Fraction*
Al	0.14286	0.07216
Co	0.28571	0.31522
Ni	0.28571	0.31392
Fe	0.28571	0.29871

Thermal treatment aim to form 3-4 phase alloy: γ, γ' + BCC(, B2)

- 1st treatment at >1000°C to get γ, γ' structure → 600°C to form B2 precipitates
  - Similar high strength alloy found from literature

Density: 7830 Kg/m^3



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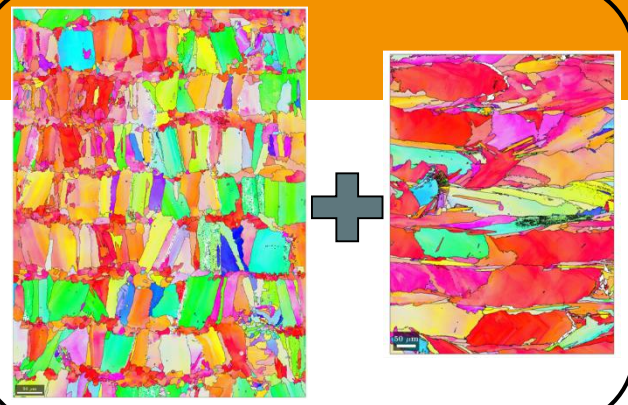
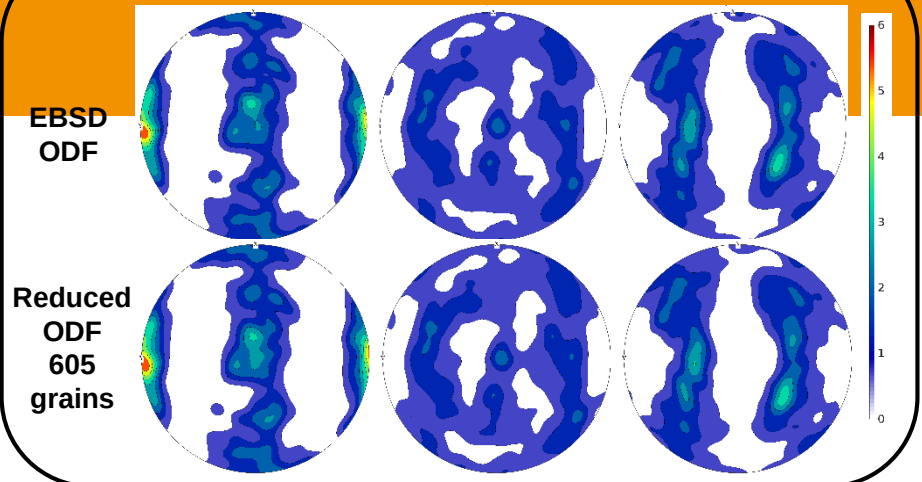
Virtual microstructure: Workflow

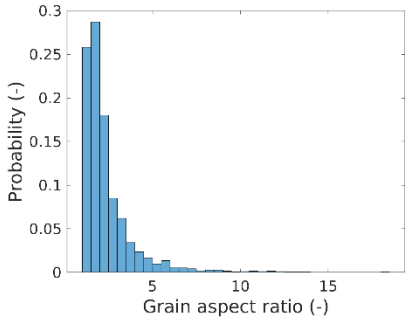
EBSD data set

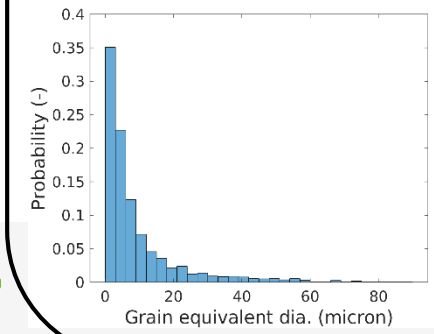


Texture module: ODF



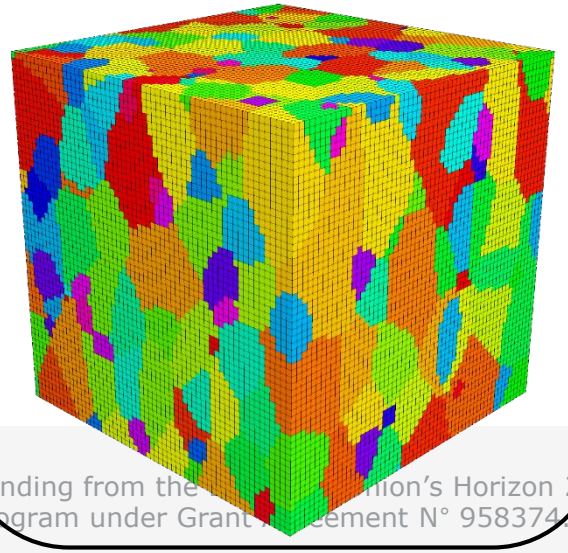
Geometry module





605 grains

Representative volume element



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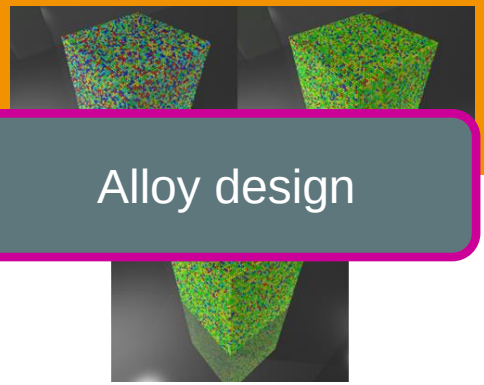
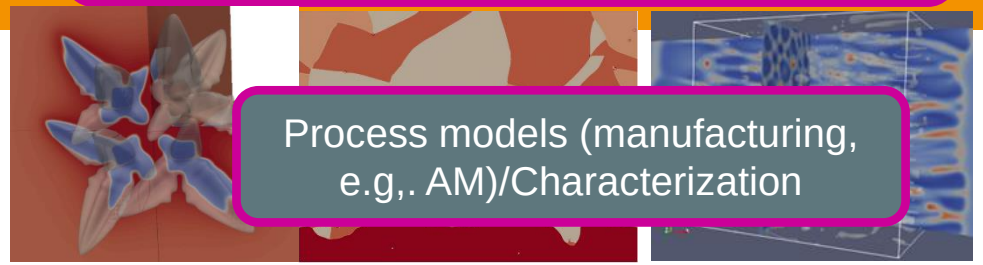
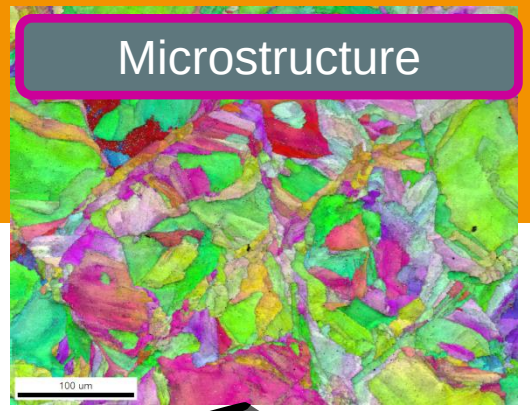


Alloy design

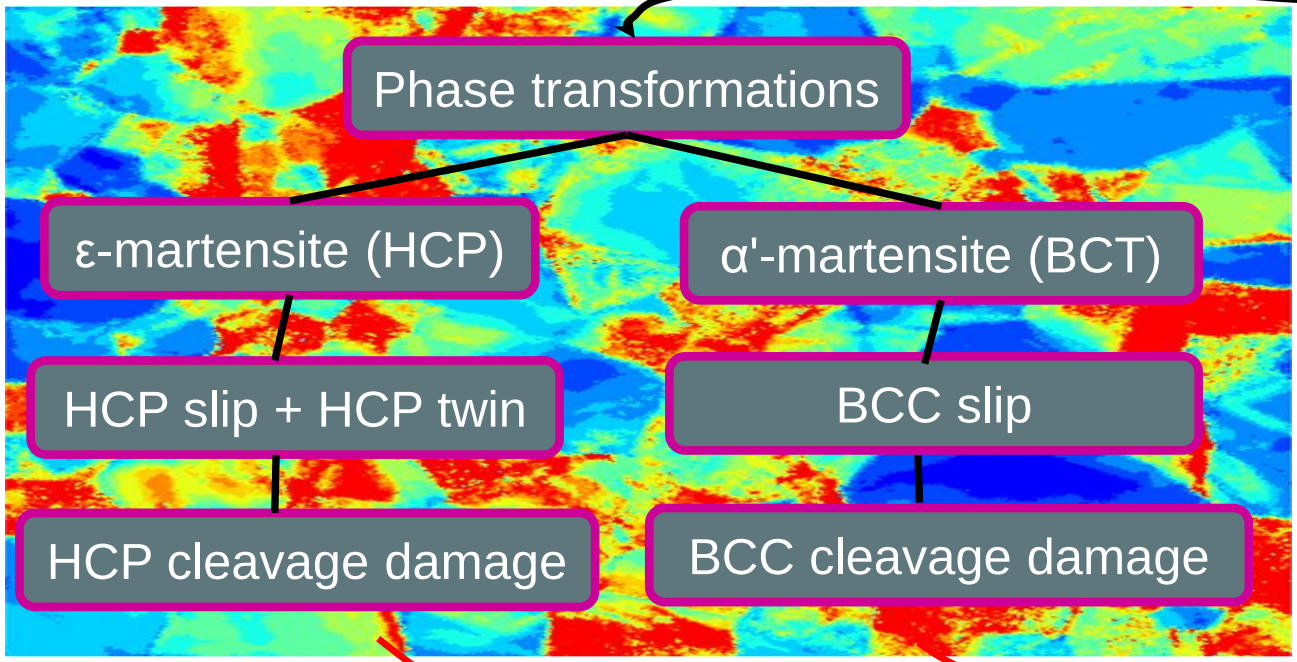
High entropy alloy material



Process models (manufacturing, e.g,. AM)/Characterization



Microstructure



Phase transformations

ε-martensite (HCP)

α'-martensite (BCT)

HCP slip + HCP twin

BCC slip

HCP cleavage damage

BCC cleavage damage

Dislocation slip

Deformation twinning

Crystal damage

Porous crystal damage

Cleavage type FCC

Material performance

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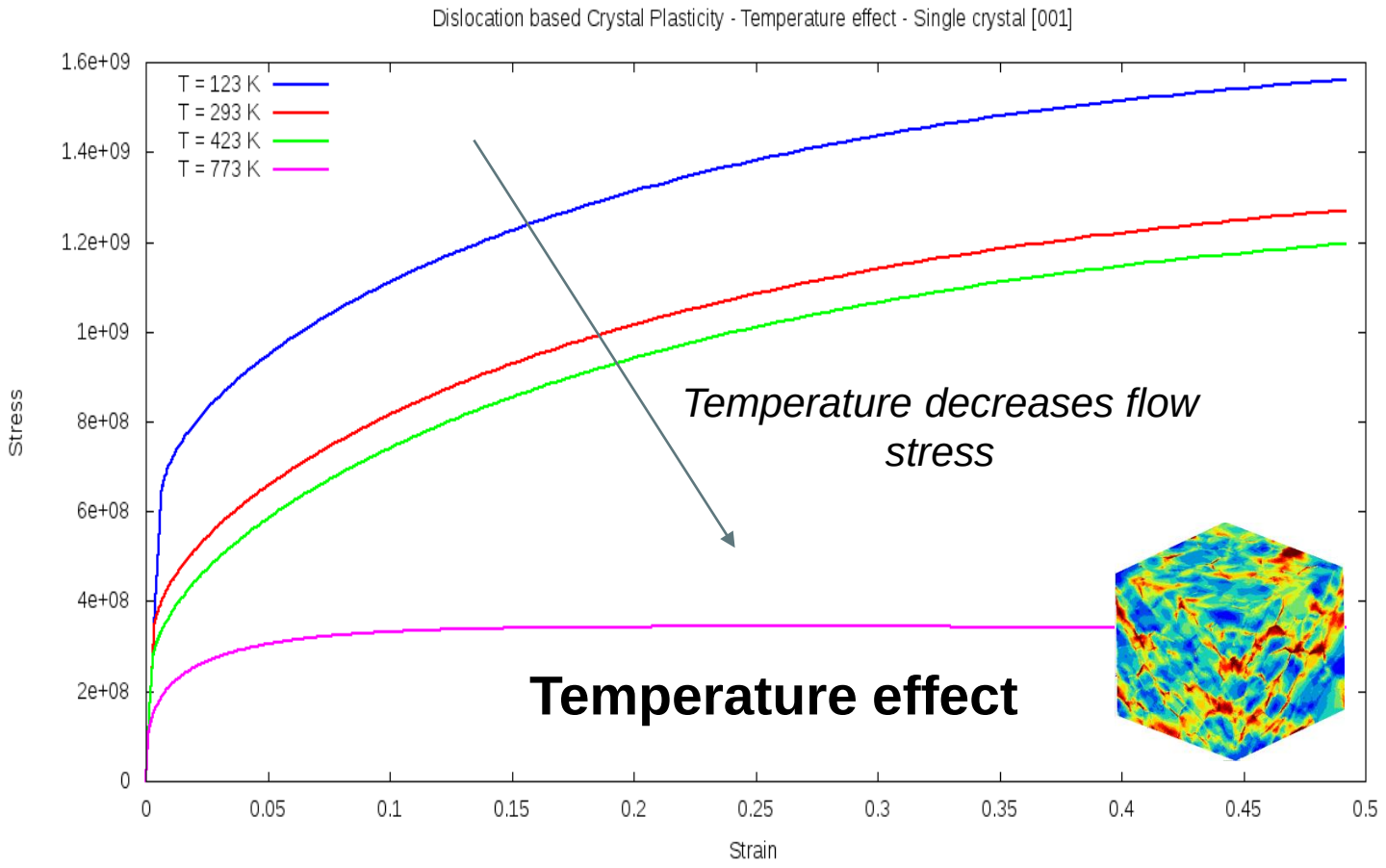
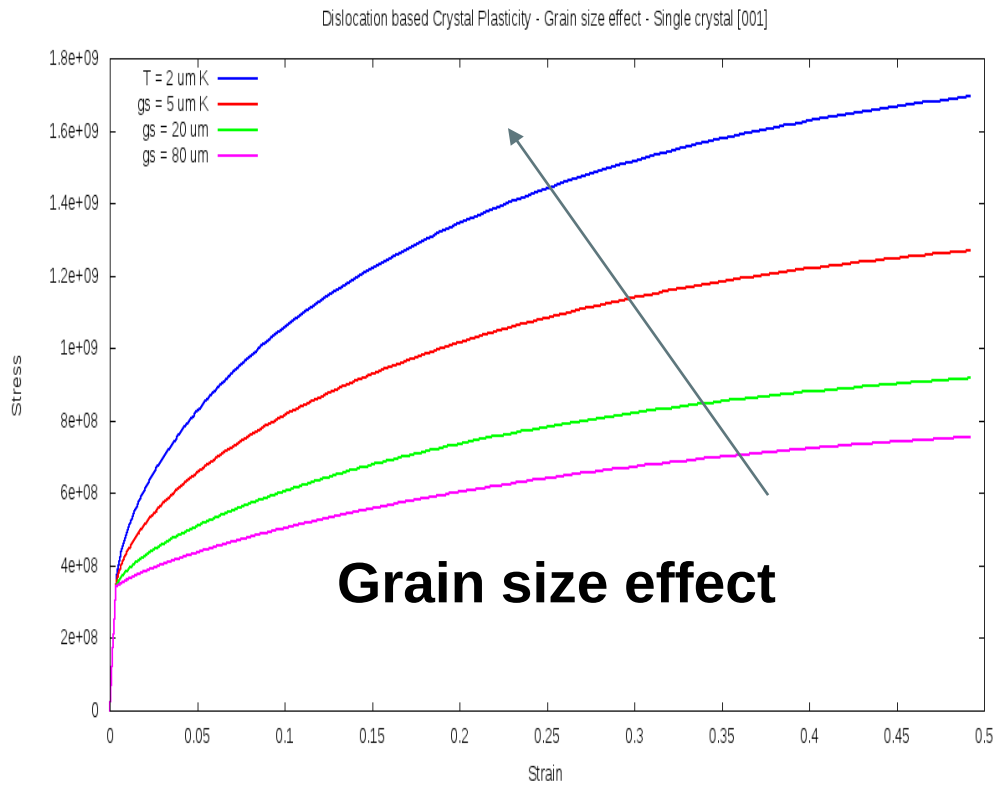
Dislocation based crystal plasticity model for HEA





Smaller grain size increases flow stress

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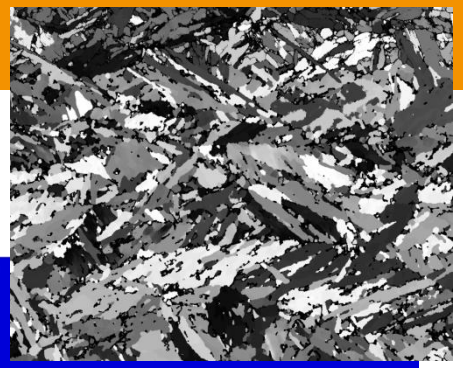
Example of microstructure design: load carrying capacity

Cumulative plastic slip



prior austenite ratio relative to reference:
a/c = 1.0 (calculated 1.5, 1.25, 1, 0.85, 0.7, 0.5, 0.25)

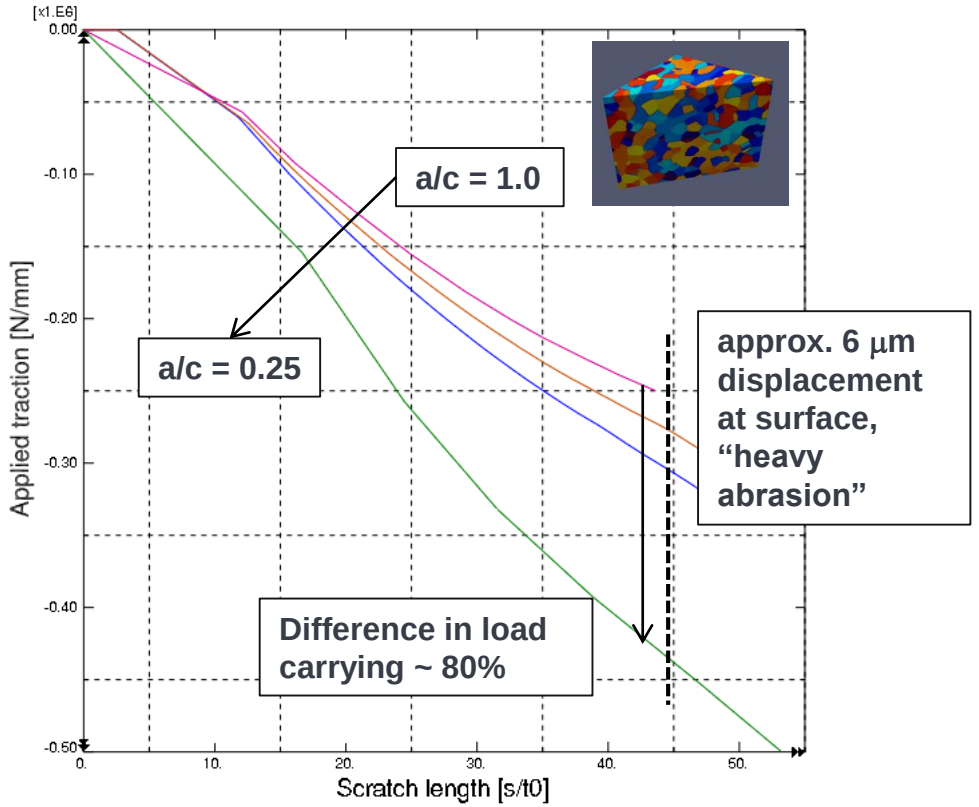
Deformation and thus most likely wear mechanism or appearance changes

a/c = 0.85

a/c = 0.7

a/c = 0.25

Two effects : i) microstructure morphology becomes more distorted and pancake like, ii) strengthening/hardening due to smaller microstructural features



Distorted structure with high prior austenite grain aspect ratio:
1) Slip resistance greater due to morphology,
2) Maximum slip localized to smaller material volume,
3) Hardening increases load carrying capacity.

Thank you!

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