COMPUTER ASSISTED DESIGN OF COMPLEX METALLIC ALLOYS

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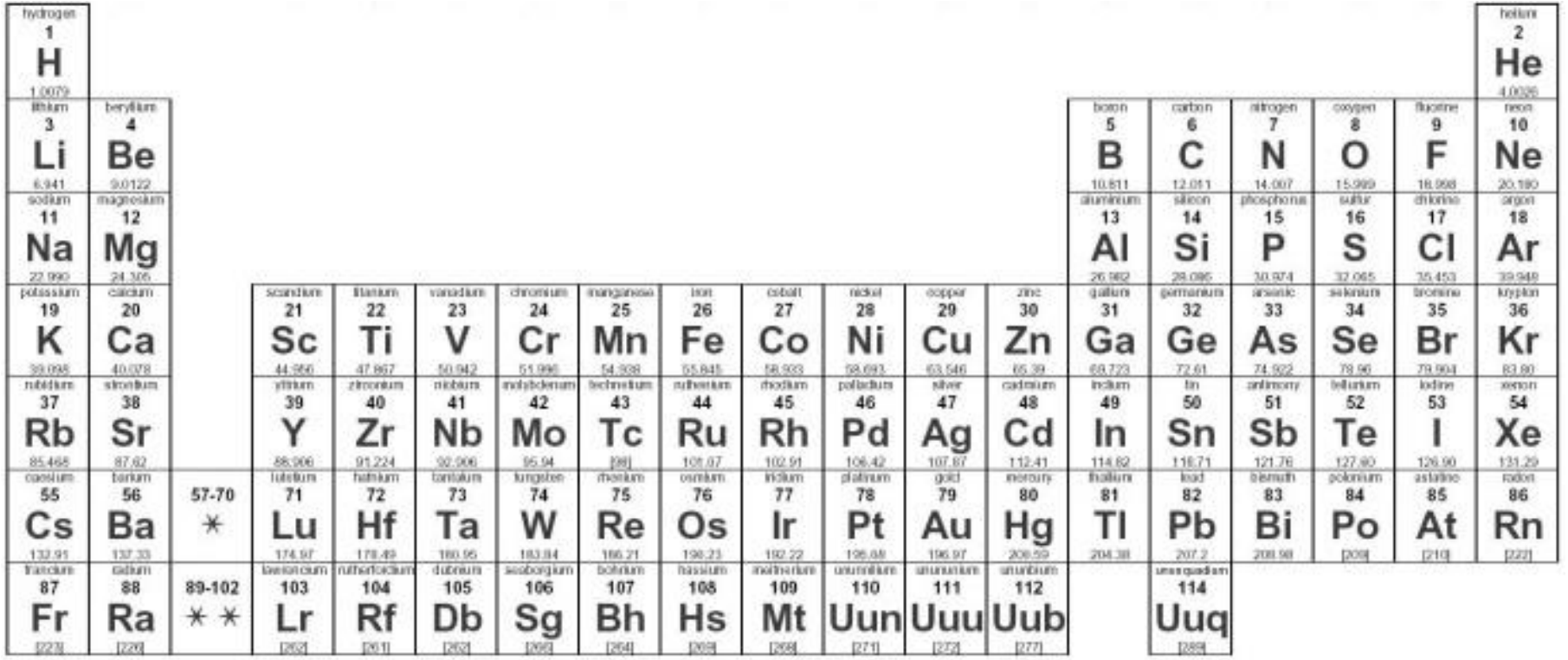
Metallic alloy design: the playground



Metallic alloy design: the playground

Bronze

~ 5000 years ago

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca		Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr		Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	57-70	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	89-102	Lr	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub		Uuq				

Metallic alloy design: the playground

Iron & Steel

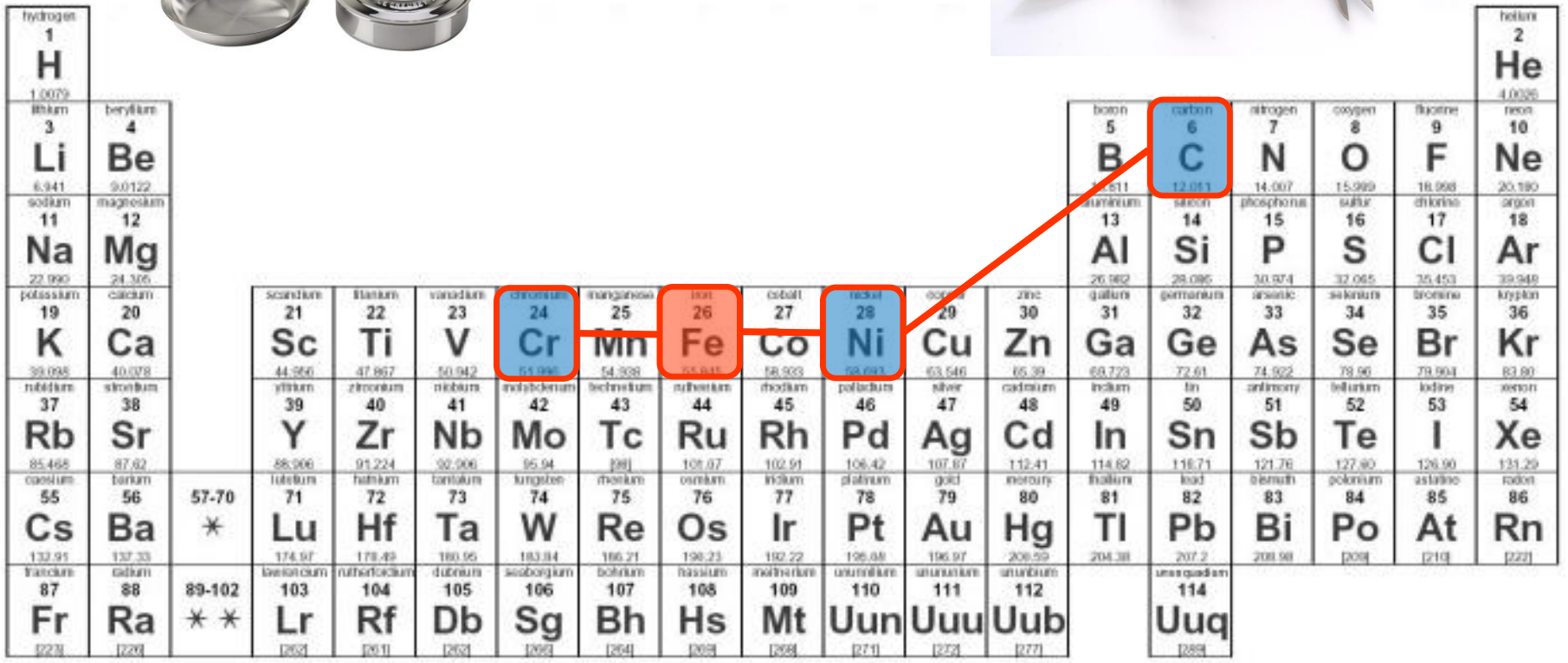
~ 3000 years ago

hydrogen 1 H 1.0079																	helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122											boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305											aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 * *	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnilium 110 Uun [271]	unununium 111 Uuu [272]	ununbium 112 Uub [277]		ununquadium 114 Uuq [289]				

Metallic alloy design: the playground

Stainless steel

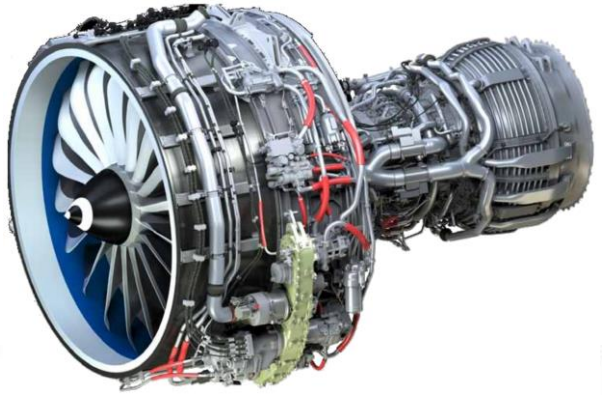
1920s



Metallic alloy design: the playground

Superalloys

1930s



hydrogen 1 H																	helium 2 He
lithium 3 Li	beryllium 4 Be											boron 5 B	carbon 6 C	nitrogen 7 N	oxygen 8 O	fluorine 9 F	neon 10 Ne
sodium 11 Na	magnesium 12 Mg											aluminium 13 Al	silicon 14 Si	phosphorus 15 P	sulfur 16 S	chlorine 17 Cl	argon 18 Ar
potassium 19 K	calcium 20 Ca	scandium 21 Sc	titanium 22 Ti	vanadium 23 V	chromium 24 Cr	manganese 25 Mn	iron 26 Fe	cobalt 27 Co	nickel 28 Ni	copper 29 Cu	zinc 30 Zn	gallium 31 Ga	germanium 32 Ge	arsenic 33 As	selenium 34 Se	bromine 35 Br	krypton 36 Kr
rubidium 37 Rb	strontium 38 Sr	yttrium 39 Y	zirconium 40 Zr	niobium 41 Nb	molybdenum 42 Mo	technetium 43 Tc	ruthenium 44 Ru	rhodium 45 Rh	palladium 46 Pd	silver 47 Ag	cadmium 48 Cd	indium 49 In	tin 50 Sn	antimony 51 Sb	tellurium 52 Te	iodine 53 I	xenon 54 Xe
caesium 55 Cs	barium 56 Ba	57-70 *	hafnium 72 Hf	tantalum 73 Ta	tungsten 74 W	rhenium 75 Re	osmium 76 Os	iridium 77 Ir	platinum 78 Pt	gold 79 Au	mercury 80 Hg	thallium 81 Tl	lead 82 Pb	bismuth 83 Bi	polonium 84 Po	astatine 85 At	radon 86 Rn
francium 87 Fr	radium 88 Ra	89-102 * *	lawrencium 103 Lr	rutherfordium 104 Rf	dubnium 105 Db	seaborgium 106 Sg	bohrium 107 Bh	hassium 108 Hs	meitnerium 109 Mt	unnilunium 110 Uun	unnilunium 111 Uuu	unnilbium 112 Uub		ununquadium 114 Uuq			

Combinatorial explosion & improvement margin

50 elements, 50 levels of concentration ~ 10^{85} alloys

Number of alloys produced characterised to date ~ 10^{6}

Wide improvement margin

but the trial-and-error approach is impractical

→ modelling

Is modelling alone enough?

If one prediction took one Planck second ($5.39e^{-44}$ s)

10^{85} x $5.39e^{-44}$ = **~ 10^{24} the age of the Universe**

Modelling of alloy properties

An **exhaustive** theoretical description **does not exist**: the problem is too complex

Numerous parameters and interactions:
composition, manufacturing routes, microstructural features, deformation mechanisms…

Combinatorial metallurgy = combinatorial explosion + complex metallurgy

To predict microstructure:
Computational thermodynamics
CALPHAD

To predict « unmodellable » properties:
Non-linear, non-parametric regression method
Gaussian processes (aka Kriging)

To screen the search space:
Non-exhaustive search method
Genetic algorithms

Nickel-based single crystal (SX) superalloys for turbine blades

Creep life modelling

1963 lines, 612 SX alloys

(from patents)

Predictive error : ~ 10%

Search

300,000,000 potential alloys

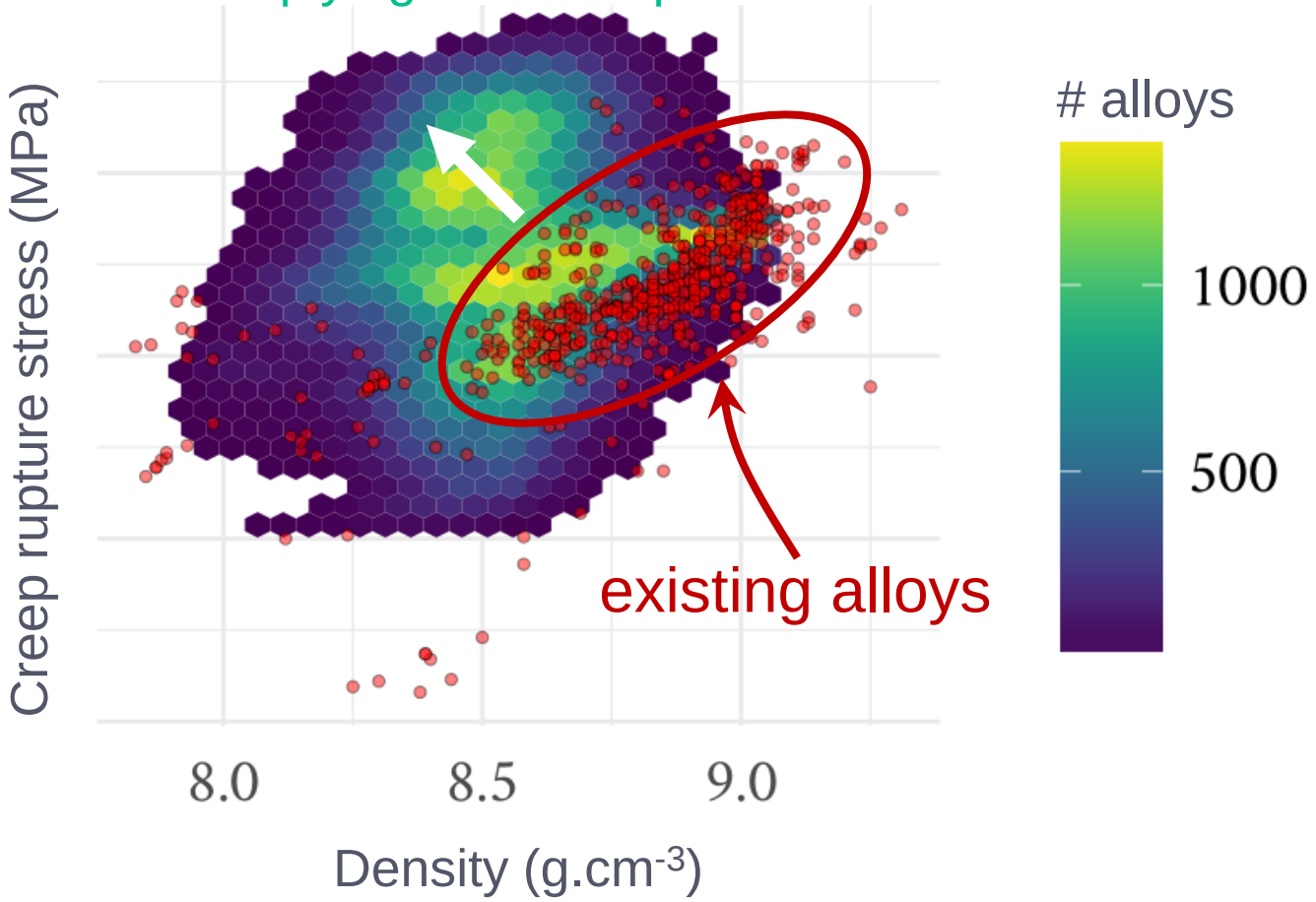
Criteria: creep life, density, stability

50 days of evaluation

50,000,000 equilibria computed

200,000 alloys

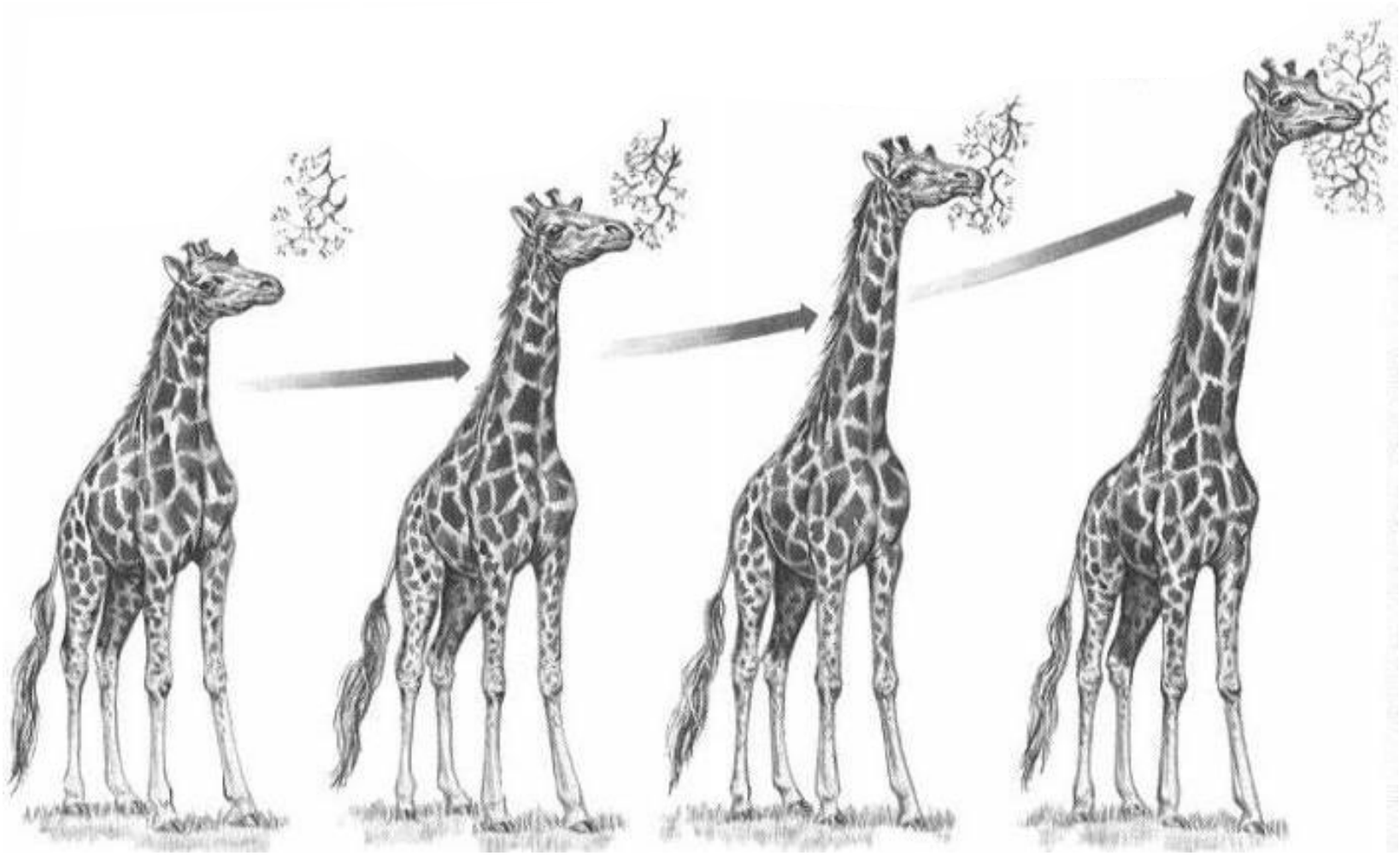
complying with the specifications



What about spaces larger than 300,000,000 feasible alloys?

Principles of genetic algorithms

Nature-inspired **genetic** manipulation



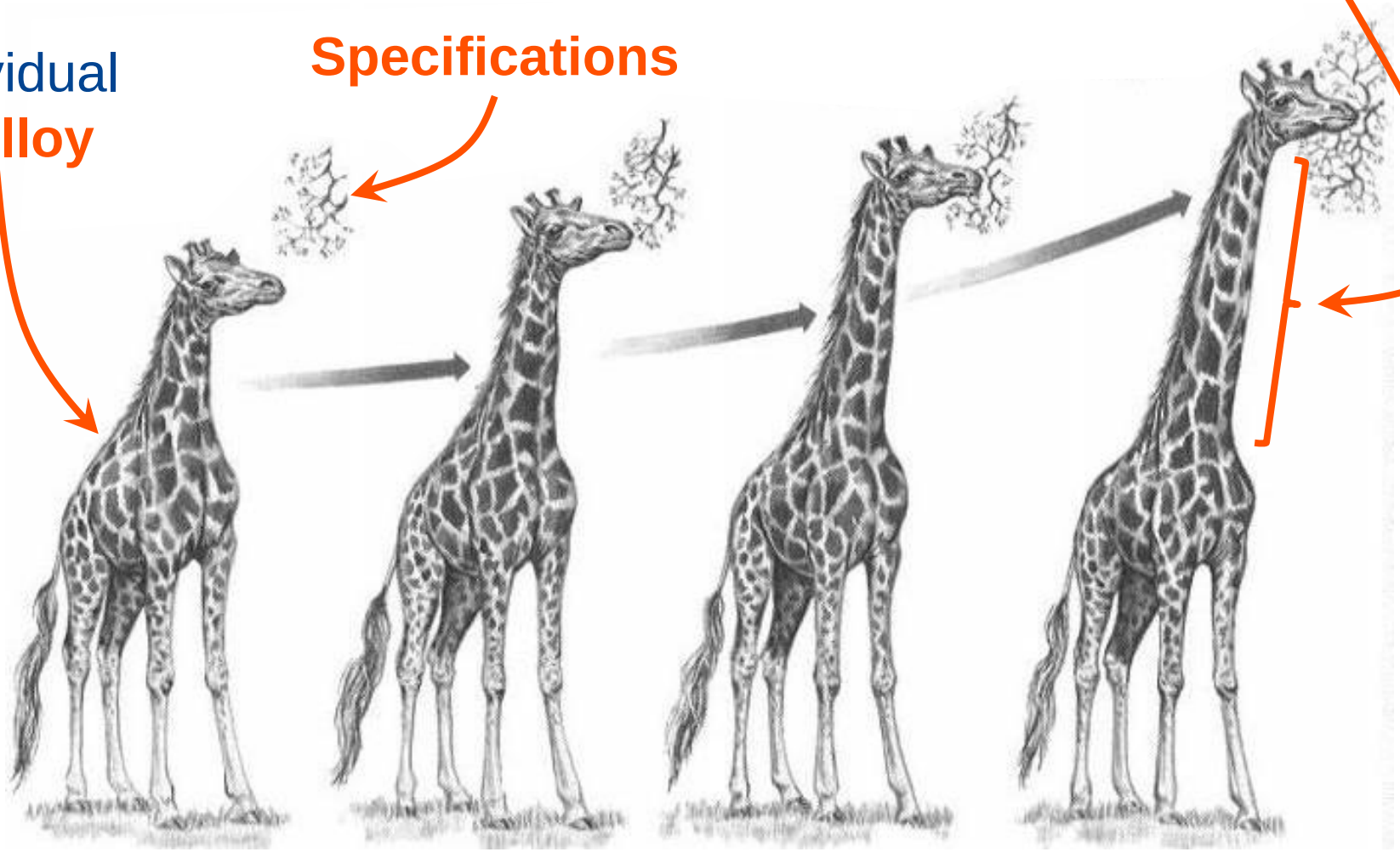
Principles of genetic algorithms

Application to alloy design

Performance
= **Properties**

Individual
= **Alloy**

Specifications

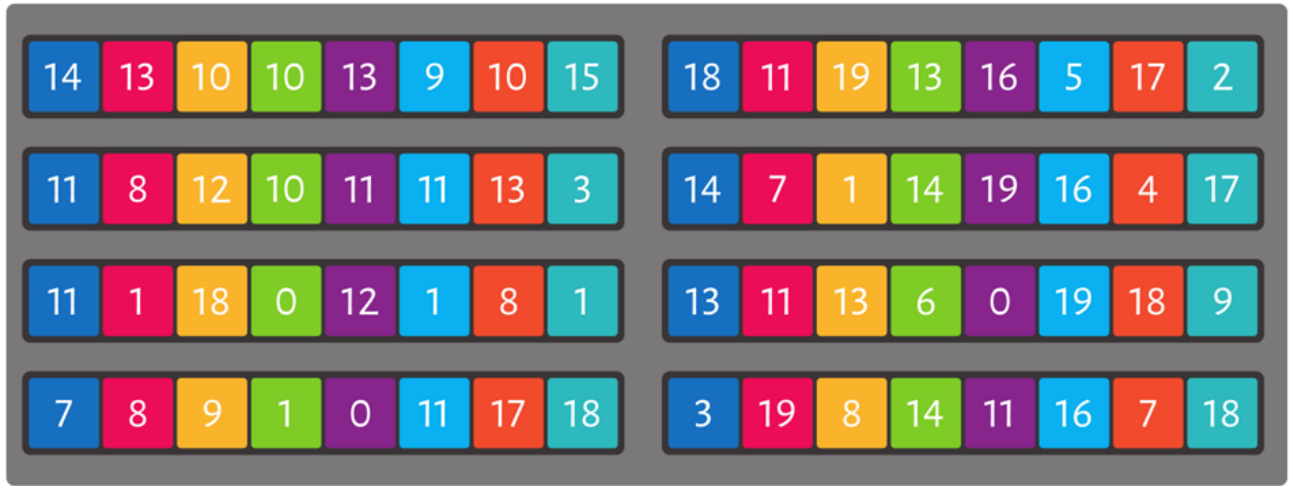


Principles of genetic algorithms

1 **alloying element** = 1 **gene**

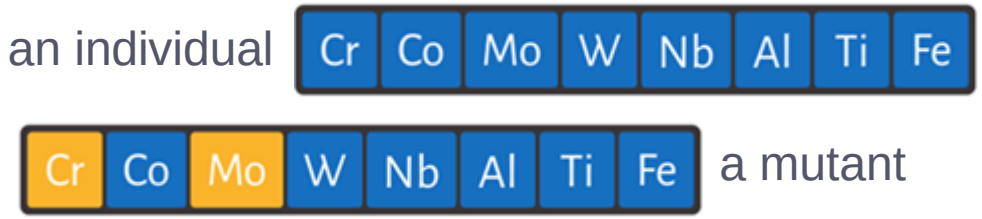
1 **alloy** = 1 **individual** = 1 group of genes

1 **population** = 1 group of **alloys**



Reproduction

Mutation



Wrought nickel-based superalloys for turbine disks

Property modelling

UTS & YS: 1928 lines

CRS: 1964 lines

(from literature)

Predictive error < 10%

Criteria

maximising

UTS, YS, CRS, forgeability

corrosion resistance, stability

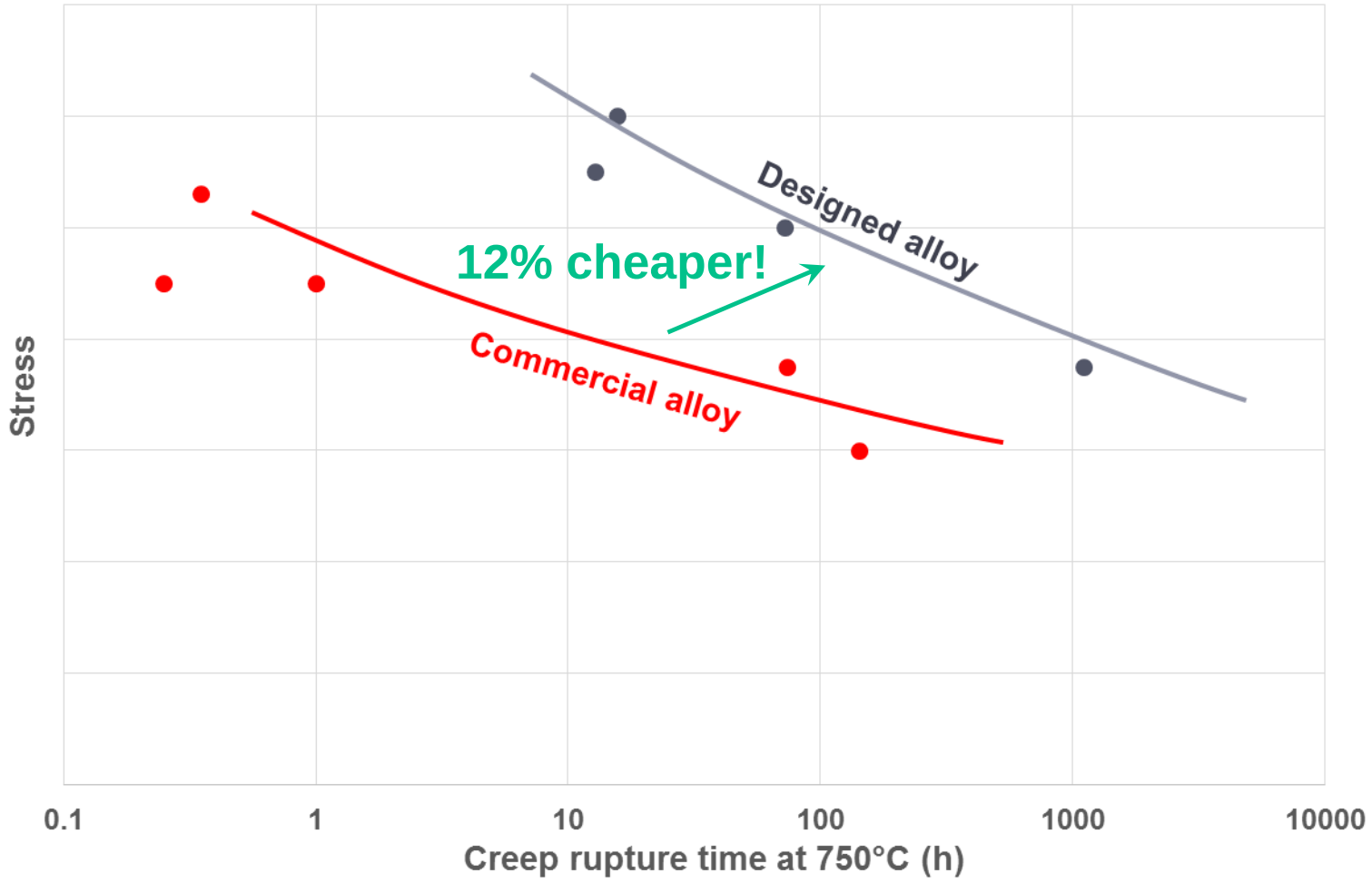
minimising

cost

density

~ 100 h of computations

~ 4000 optimal alloys → 1 tested



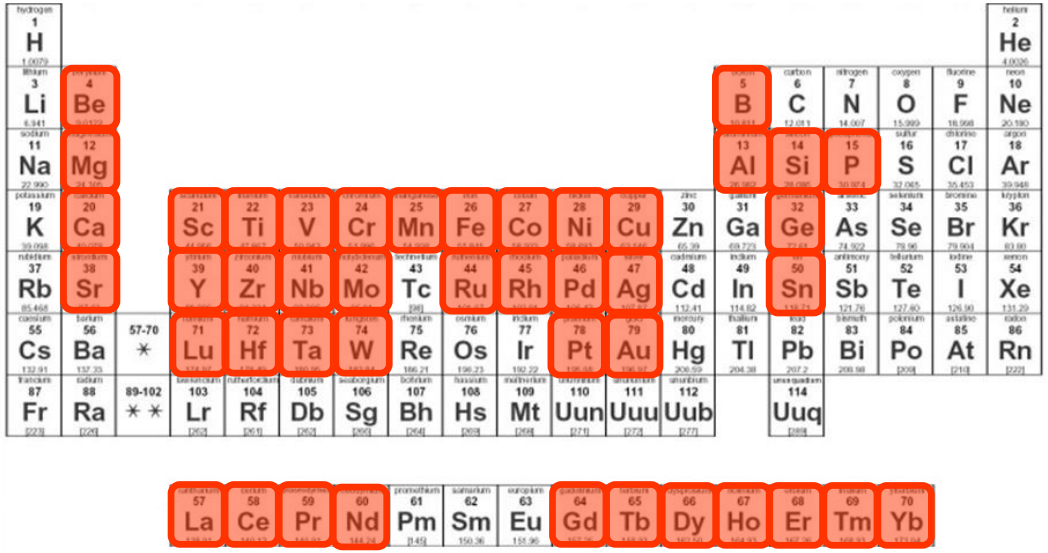
A. Deschamps *et al.* Comptes Rendus Physique (2018)

High entropy alloys

At least **5 elements**

Between **5** and **35 at.%** each

A **single solid solution**



How to predict the formation and stability of a single solid solution?

UNIVERSITY OF CAMBRIDGE

Criterion P_{IF} : statistical analysis on various physicochemical parameters

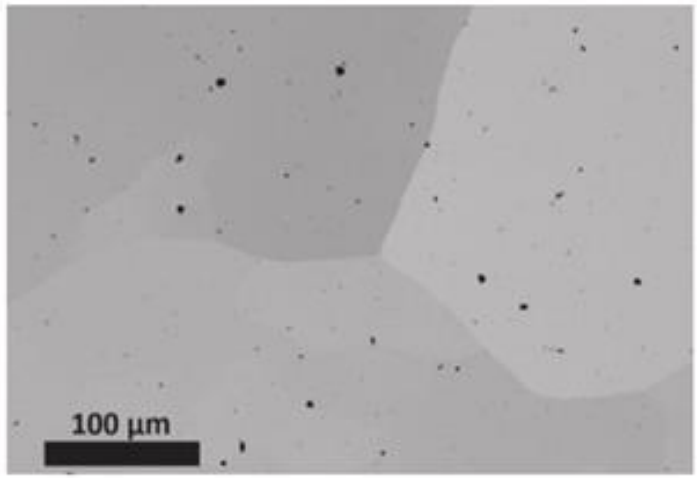
(atomic radius, interatomic distance, bulk modulus, electronegativity, valence, …)

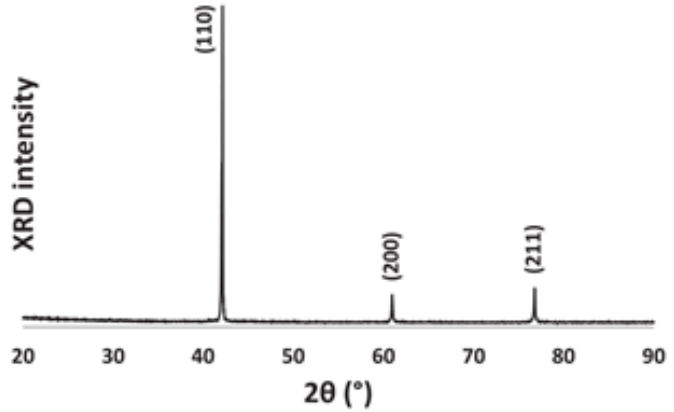
F. Tancret *et al.* Materials & Design 115 (2017) 486–497

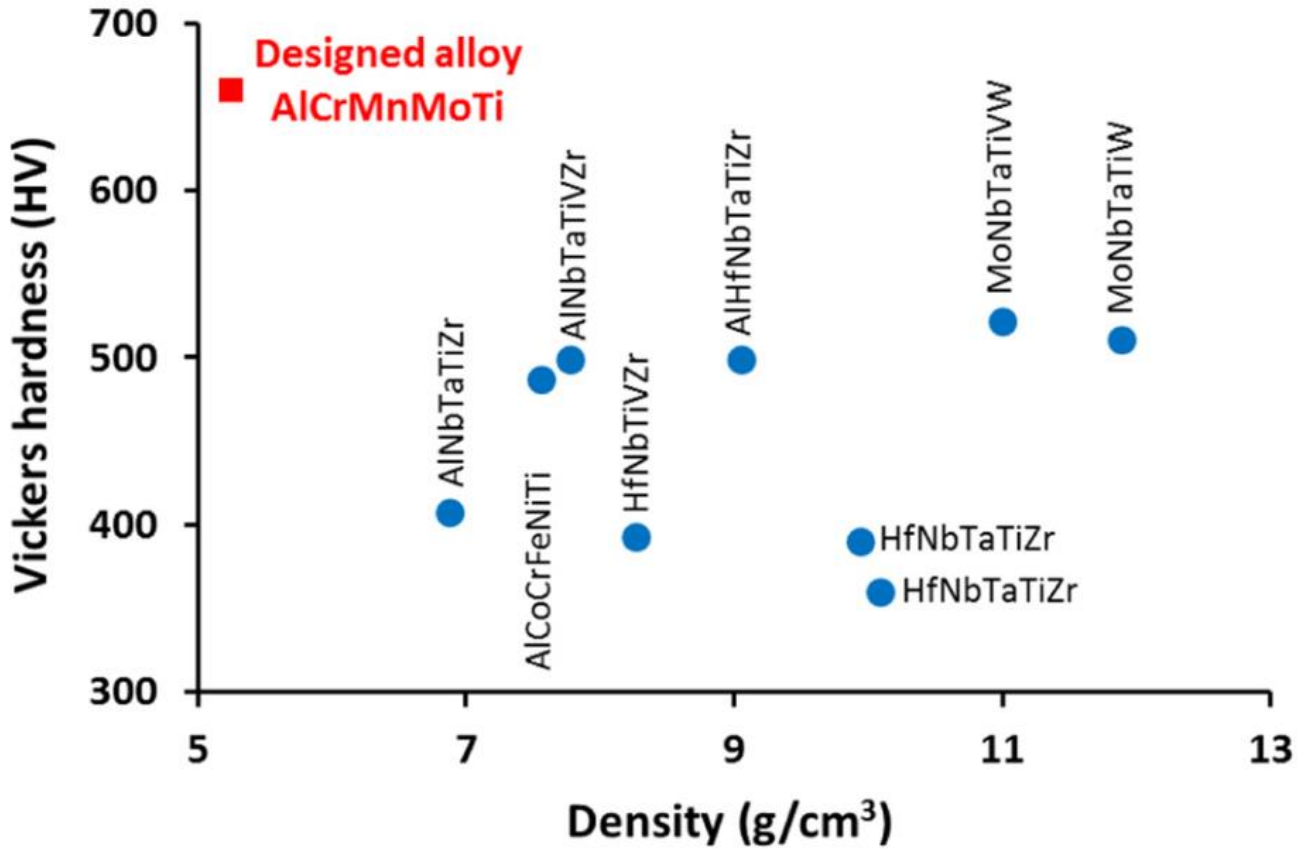
High entropy alloys

Criteria: probability P_{IF} – density – solid solution hardening

Experimental validation: $Cr_{37}Al_{31}Ti_{19}Mn_7Mo_6$







E. Menou *et al.* Scripta Materialia 156 (2018) 120–123

Merci pour votre attention !