COMPUTER ASSISTED DESIGN OF COMPLEX METALLIC ALLOYS

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Metallic alloy design: the playground

tydrogen 1 H																		2 He
athium 3	beryfiam 4												boton 5	carbon 6	nitrogen 7	cxygen 8	fluorine 9	10
Li	Be												в	C	N	0	F	Ne
6.941	9.0122												10.811	12.011	14.007	15.999	18.998	20.190
sodium 11	magnesiam 12												auminium 13	14 sticon	phosphonia 15	16	entorine 17	argon 18
Na	Mg												AI	Si	P	S	CI	Ar
22.990	21.305		S		0				S			<i>i</i> – – – – – – – – – – – – – – – – – – –	26,962	28.095	30.974	32,065	35,453	39,948
potsssium 10	20 20		scandure 21	11anam 22	vanadam 23	24	nanganisia 25	26	27	28	copper 20	2me 30	galuo 31	germanium 32	arsenic 33	seknun 34	arcmine 35	krypton 36
1Z	C-		6.	T	N/	<u> </u>	B.6	E.	c'-	ALC:	C	7.	0-	0-	A -	0.0	D	1/m
n	Ca		SC	11	V	Ur	win	ге	CO	NI	Cu	zn	Ga	Ge	AS	Se	Br	nr
39.095	40.078		44:966	47.867	50.942	51.996	54.938	65.845	58,903	58.693	63,546	65.39	68,723	72.61	74.922	78.96	78.904	83.90
37	38		39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr		Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	1	Xe
85.465	87.62		88.906	91.224	92.906	95.94	[98]	10t.07	102.91	106.42	107.87	112.41	114.62	116.71	121.76	127.60	126.90	131.29
55	56	57-70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Ce	Pa	×	Lu	LIF	Ta	14/	Pa	Oc	lr.	Dt	Δ	Ha	TI	Dh	Di	Do	Λ+	Dn
US	Dd	A	Lu	п	Id	VV	Re	US	ш	PL.	Au	пg		PD	DI	FO	AL	KII
132.95 Yatchre	137,33 radium		174.97 Iowioncium	178,49 ruthertoxclum	dubrium	septoraium	186.21 bohrum	198,23 hassium	192.22 methadure	196.68 unumnhum	196.97 WHOMING	206.59 ununbium	204.38	207.2	208.98	208	1210	222
87	88	89-102	103	104	105	106	107	108	109	110	111	112		114				
Fr	Ra	**	1 r	Rf	Dh	Sa	Bh	Hs	Mt	Hun	thui	Hub		Uur				
17273	1220		12621	DOT	12621	000	(264)	Dia	12691	12711	1273	12771		1289				



Metallic alloy design: the playground

hydrogen 1 H		ß	Ĩ		1		~ 50	Bro 000 y	o nze rears	e ago								^{beilum} 2 He
ithim 3	4 Be												5 B	e C	ntrogen 7 N	8 O	9 F	10 10 Ne
6.941 sodium	9.0122 magnesium												10.611 aluminium	12.011 silicon	14.007 phosphorum	15.990 6480	18.998 ditionine	20,190 97901
11 No	12 Ma												13	14 Ci	15 D	16 C	17 CI	18 Ar
22.990	21.305				9								26,142	28.095	30.974	32.065	35,453	AI 39,949
19	20		scandium 21	Elantorn 22	23	chronium 24	nanganese 25	26	27	28	29	2me 30	gature 31	32	arsanic 33	selenium 34	35	krypton 36
K	Ca		Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
39.098 n.6idkm	40.078 stontum		44.956 3/Bitum	47.867 zirconkum	50.942 nicbium	51.996 nolabdenum	54.938 technetum	55.845 rubetkm	58.933 rhodium	58.093 poliadiute	its san silver	65.39 cadmium	68,723 Incilum	-72.61 In	74.922 antimony	78.96 tellurium	79.904 Iodine	R3.90 Xenon
Ph	Sr		39	40 7r	Mb	42 Mo	43 TC	P11	Ph	Pd	Ad	Cd.	In	Sn	Sh	To	53	Xo
85.465	87.62		88,906	91,224	302.006	95.94	1981	101.07	102.91	106.42	107.67	112.41	114.62	11871	121.78	127.90	126.90	121.20
caesium 55	56	57-70	71	72	tantalum 73	tungsten 74	rbenkm 75	76	ridium 77	platinum 78	00kl 79	80	fialium 81	82	83	90kmium 84	astatine 85	radon 86
Cs	Ba	*	Lu	Hf	Та	W	Re	Os	lr	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
132.95 Yatchre	137,33 radium		174.97 Iowioticium	178,49 rutherfoldium	180.95 dubnium	183.84 seaborgium	166.21 bohrkm	198.23 hassium	192.22 moltharture	196.68 counnitium	196.97 шилилит	208.59 ununbium	204.38	207.2 unasquadiani	201.98	poor	1210	[227]
87	Ba	89-102	103	104 Df	105 Dh	106	107 Dh	108	109 B/I+	110	111	112		114				
12238	1220	~ ^	12621	[201]	12021	Java	[264]	100H	IVI L	[271]	1273	1277		JZ89				

MIN Street



Metallic alloy design: the playground

Iron & Steel ~ 3000 years ago		helium 2 He
ittiam beydam attop attop 7	gen oxygen fluor	ne neon 10
Li Ba		No
6.941 9.0122 10.811 12.011 14.0	07 15.999 18.9	98 20,190
solum magnesium 11 12 13 14 15	hona sultur dhion 5 16 17	na argon 18
Na Ma	SC	1 Ar
22 190 24 305 25 192 28 085 30 19	37.065 35.4	53 39.949
potassium calcum scandum flantum vanadum chromium nangarose ion cubalt netoe oppor zinc gallum permanum arsen	nic salanium brom	ine krypton 346
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge A	SA B	r Kr
Salas 40.078 41.977 51.987 50.992 51.996 51.988 55.418 55.98 53.546 55.58 59.773 77.61 71.97	3 SC D	0.1 R3.00
nöldum stonbun yittum zeronium nölzöum nölzökenum jechnetium nölseken hodium poliidum silver cadmium inclum in artime 37 38 30 40 41 42 43 44 45 46 47 48 40 50 51	ony telurium lodir	ve xemon
Ph Sr V 7r Nh Mo To Pu Ph Pd Ag Cd In Sn St		Vo.
85.465 87.62 ROLE 01.224 07.966 95.94 898 106.07 107.07 107.07 117.07 112.41 114.62 116.71 114.62	76 127.60 1260	131 29
coostum tertum lidetum hamam toritaum langsten mentam osmiam lidetum gold mercury fination load bleme	uth polonium astat	100 10001
Co Po X Lu Uf To W Po Oo Ir Dt Au He TI Dh P		+ Dm
CS Da * LU HI IA W KE US II PI AU HG II PD D	POA	I KI
Tatolan odum lavisticum niteriocium dubrium seeborgium bolmum hassium molherium unumlum unumlum unumlum unumlum unumlum unumlum	and head I but	I loss
F_r Do $\times \times$ Lr Df Db Sa Db Ho Mt Hum Hum Hum		



Metallic alloy design: the playground

hydrogen 1 H						30	Sta	inle 19	92 0s	ste	el	0					and a second	^{bellars} 2 He
athian a	berylikm	Ê										1	boton	carbon	aitrogen	cosygen	fluorine	10025
1 i	Ro												R	ċ	N	Ô	F	No
6.941	9.0122												5611	12.011	14.007	15.999	18,998	20,180
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Na	Ma												AI	Si	P	S	CL	Ar
22,990	21.305		s		0						-		26,962	28.095	30.974	32,065	35,453	39,949
potassium 19	calcium		scandum 21	Banara 22	vanadium 23	24	manganese 25	26	27	28	29	2002 30	gature 31	germanium 32	arsonic 33	seknium 34	tronine 35	krypton 36
K	Ca		Sc	Ti	V	Cr	Min	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
39.098 n.644m	40.078 stontum		44:956 vitrium	47.867 zirconium	50.942 niobium	nifebolerum	54.938 technistum	national and	58,933 rhodium	polisitum	63,546 silver	65.39 cadmium	68,723 Inclum	72.61 tin	74.922 antimony	78.96 tellurium	79.904 Iodine	83.90
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Rb	Sr		Y	Zr	Nb	Mo	TC	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te		Xe
85.468 caesium	87.62 tarium	-	- 88:000 Tubelom	91.224 https://	32.906 tontolum	95.94 tungstee	[98] (thetkee	10t.07 osmiam	102.91 Midlum	106.42 diatinum	107.87	112.41 mercury	114.62 ftolium	118.71 kod	121.76 bismuth	127.90 polonium	126.90 astatine	131.29 Fador
55	56	57-70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ba	*	Lu	Hf	Та	W	Re	Os	lr	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
132.95 Kanchan	137,33		174.97	178.49 netodiachem	180.95	. 183.84 september	186.21 bolidum	198.23 basslum	192.22 motharture	196.68	196.97	208.59	204.38	207.2	208.98	209	1210	[227]
87	88	89-102	103	104	105	106	107	108	109	110	111	112		114				
Fr	Ra	**		Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub		Uuq				

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Metallic alloy design: the playground

frydrogen 1 H							Su	per 193	allo 30s	oys								^{holium} 2 He
1.0079 Bhlum 3	terylium 4											ľ	boron 5	6	nitrogen 7	000ygeri 8	fluorine 9	4.0026 resin 10
6.941	Be 9.0122												B	C 12.041	N 14.007	O 15.999	18,998	20,180
sodium 11	magnesium 12												13	14	phosphone 15	sutter 16	dhiorina 17	argon 18
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22.990 potassium	24.305 calicium 20		scandium 21	22	vanadium 23	dironium 24	1003000	26	27	28	20 (par	2002 30	galuo 31	semaneun 32	30.974 arsenic 33	32.065 seknun 34	35,453 bronine 35	39.948 Mypton 36
ĸ	Ca		Sc	Ťi	Ň	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
39.098 néidkm	40.078 strontum		44.956 vitrium	47.967 2800000	50.942 netem	S1 BM	te son	TANKILIT	ra oro	policiture	63,546 sher	65.39 cadmium	68,723 Inclum	72.61 fin	74.922 antimony	78.96 tellurium	79.904 lodine	83.90 xemon
37	38		39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
RD	Sr		Y		ND	MO	IC	Ru	Rn	Pa	Ag	Ca	In	Sn	SD	le	126.00	Xe
caosium 55	tarium 56	57-70	Tutetura 71	72	torntourn 73	Autostee 74	75	osmism 76	indum 77	platinum 78	9083 79	mercury 80	falian 81	kod 82	benuth 83	polonium 84	astatine 85	Fadort 86
Cs	Ba	*	Lu	Hf	Та	W	Re	Os	Ir	Pt	Au	Ha	TI	Pb	Bi	Po	At	Rn
132.95 Tatchre	137,33 radium		174.97 Iowisticum	Invited Sector	digraum	Leaderstein	106.71	198:23 hassium	192.22 Ineltherture	196.68 gourollure	196.97 JIDUOUTUM	208.59	204.38	207.2	201.98	12008	1210	[227]
87	88	89-102	103	104	105	106	107	108	109	110	111	112		114				
Fr	Ra	**		Rf	Db	Sg	8h	HS	INT	JUUN	Uuu	Uub		Uuq				



Combinatorial explosion & improvement margin

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

Number of alloys produced characterised to date $\sim 10^6$

Wide improvement margin

but the trial-and-error approach is impractical \rightarrow modelling

Is modelling alone enough?

If one prediction took one Planck second (5.39e⁻⁴⁴ s)

 $10^{85} \times 5.39e^{-44} = ~ 10^{24}$ 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



Density (g.cm⁻³)

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



Principles of genetic algorithms

Nature-inspired genetic manipulation









Principles of genetic algorithms

1 alloying element = 1 gene

Cr

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

Cr Co Mo W Nb Al Ti Fe

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



Reproduction



Mutation											
an individual	Cr	Co	Мо	W	Nb	Al	Ti	Fe			
Cr Co Mo W Nb Al Ti Fe a mutant											



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





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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?



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

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

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

High entropy alloys

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

Experimental validation: Cr₃₇Al₃₁Ti₁₉Mn₇Mo₆



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





Merci pour votre attention !

