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[1] Tata Steel
[2] MPIE

Predicting the M_s temperature of steels with a thermodynamic based model including the effect of the prior austenite grain size

28 June 2017

GTT-Technologies meeting

* This work has been conducted in the framework of RFCS project ToolMart

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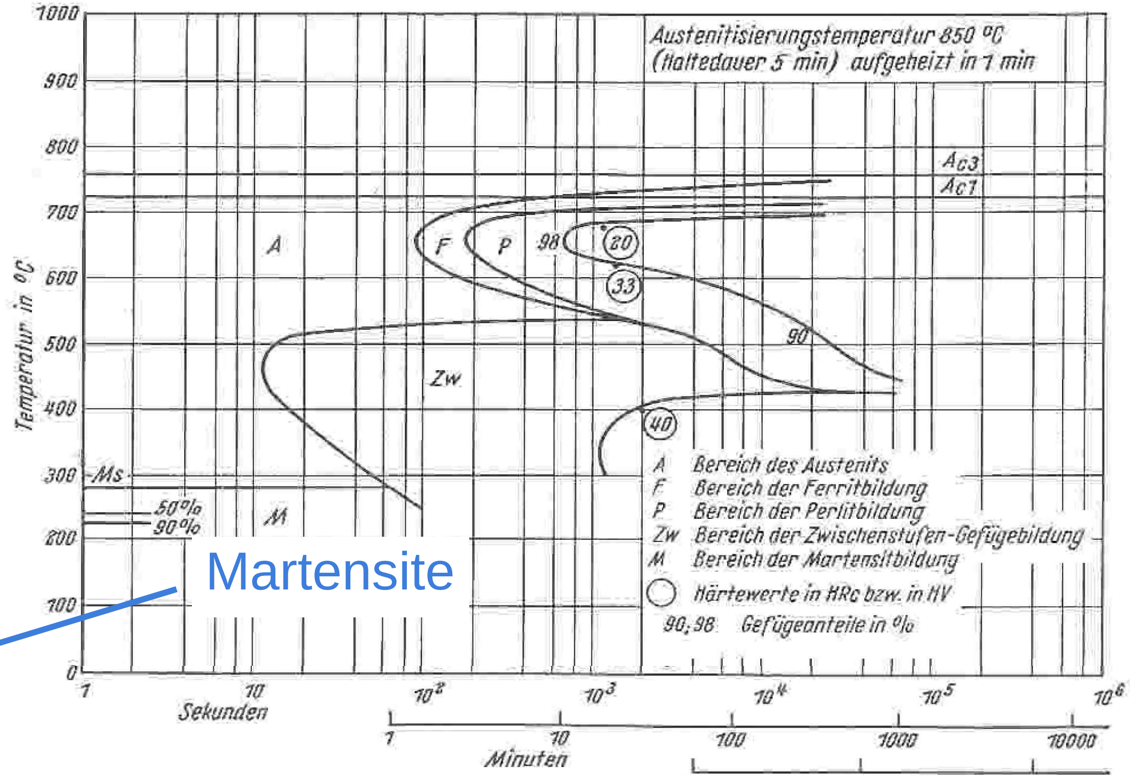
Outline

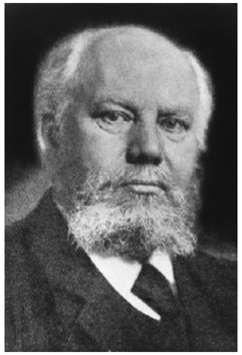
Martensite

50 CrMo 4 (SAE 4150)

Composition: 0.50% C - 0.80% Mn - 0.32% Si - 0.017% P - 0.022% S - 1.04% Cr - 0.17% Cu - 0.24% Mo - 0.11% Ni - <0.01% V Austenitized at 850°C (1562°F)



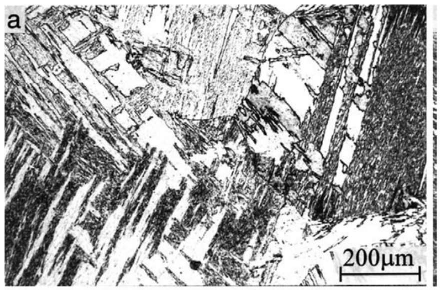
Martensite



Adolf Martens

1850-1914

Martensite start (M_s) temperature versus Carbon content



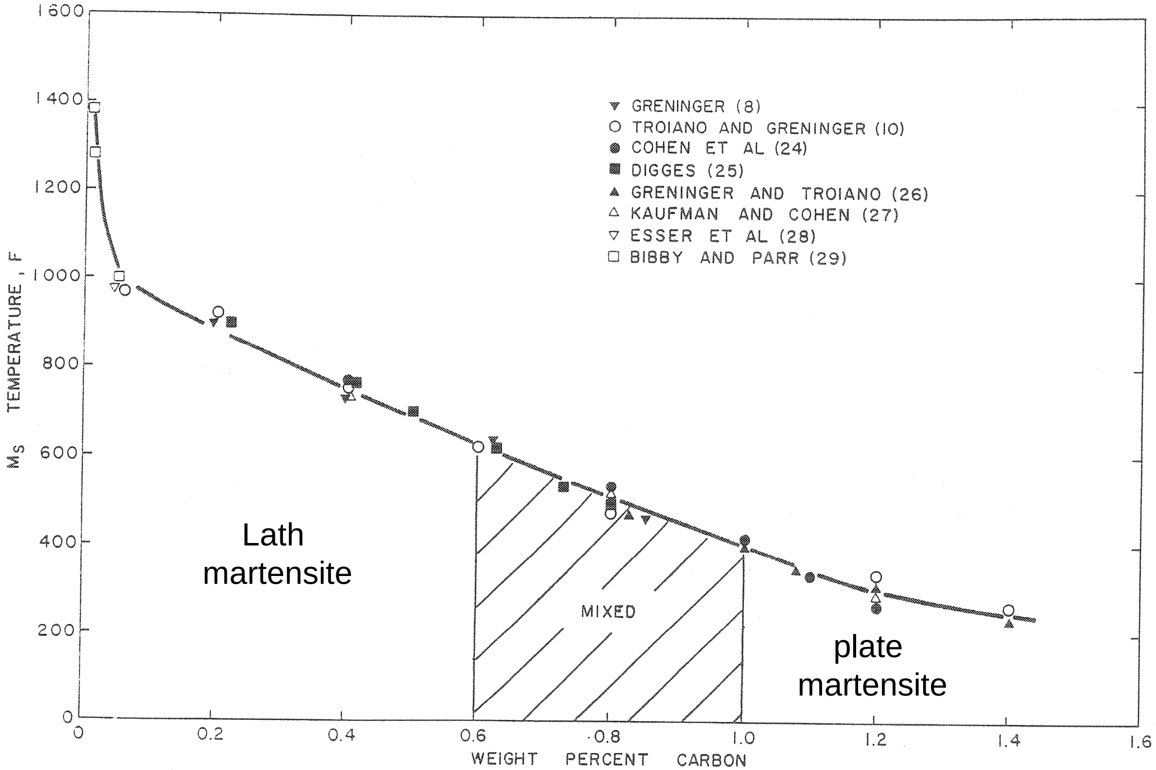
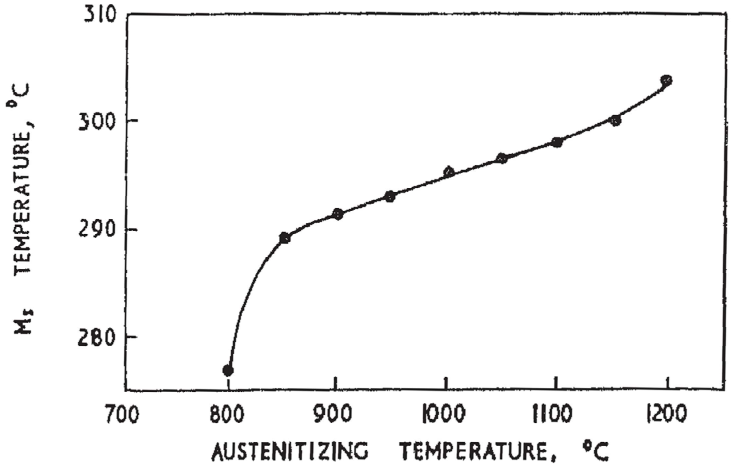


FIG. 9. Martensite transformation start temperatures (M_s) vs carbon content. The range of compositions in which the various types of martensite exist is also shown.

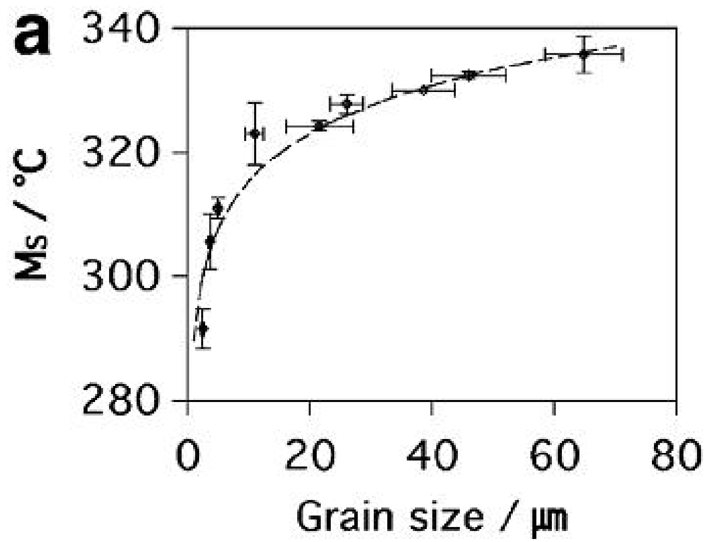
Courtesy: Marder and Krauss (1967)

Effect of Austenite Grain Size on M_s



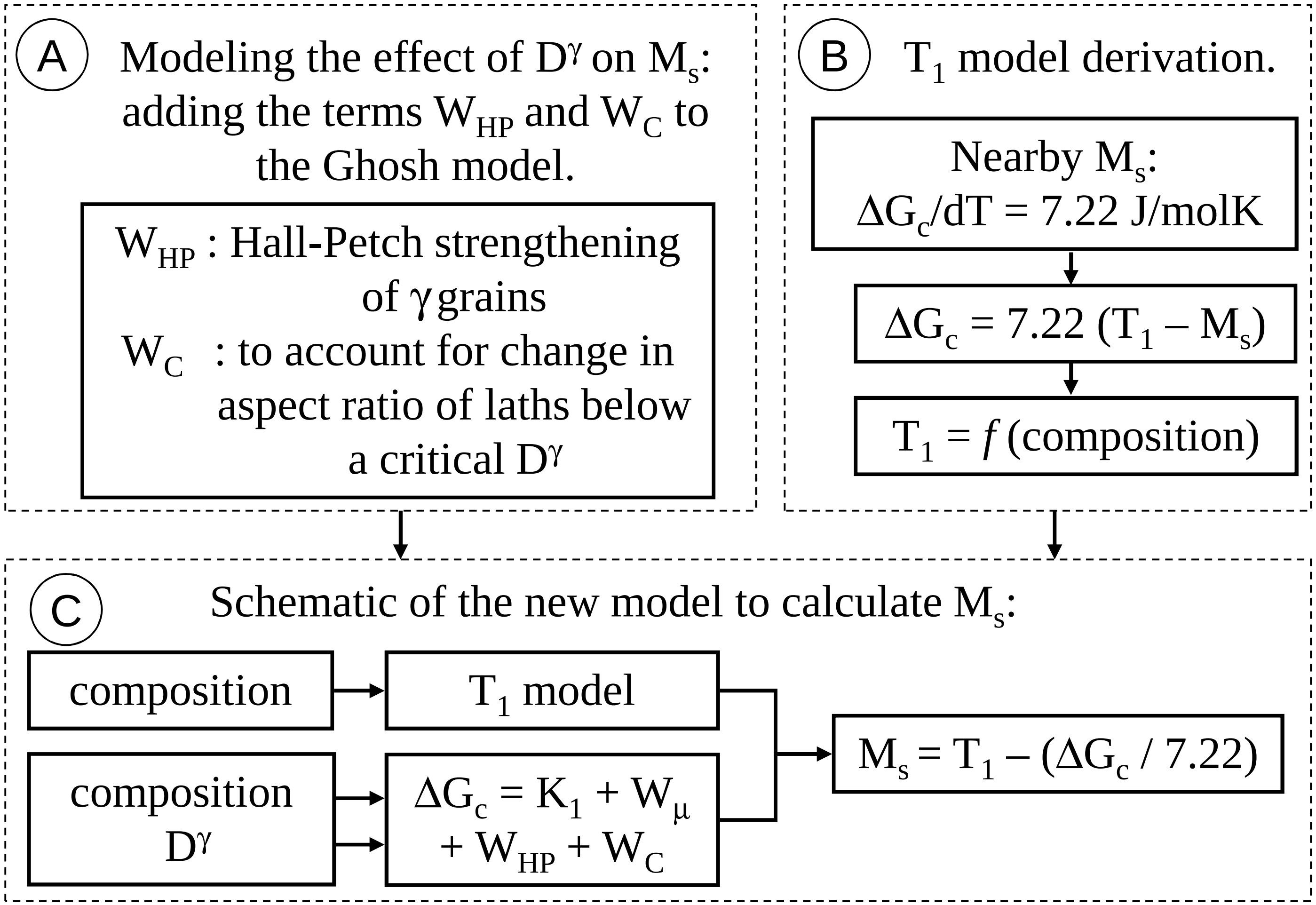
1a *Variation of M_s with austenitizing temperature for an En23 steel*

Sastri, 1965

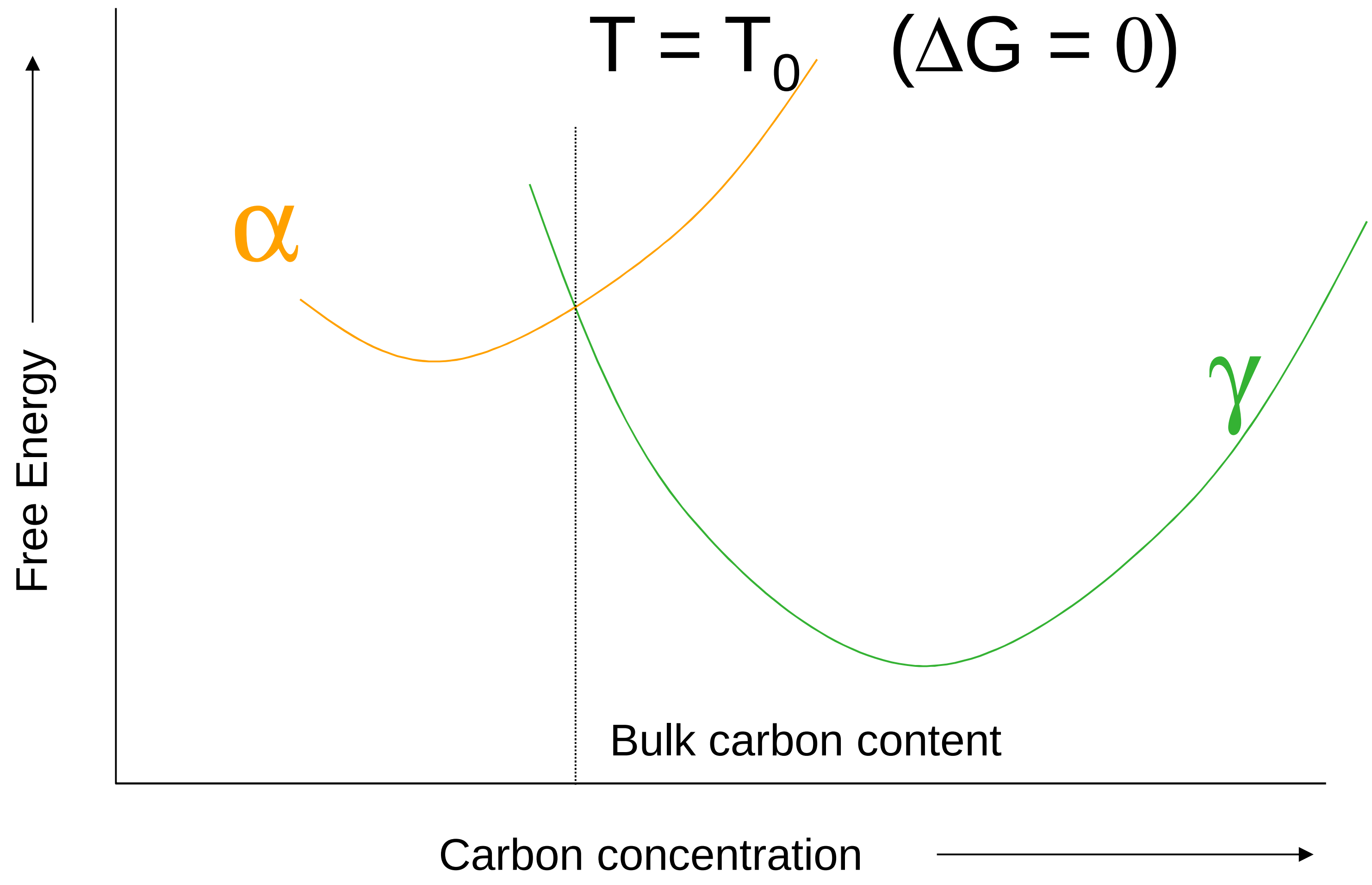


Yang, 2009

Schematic of the modeling approach

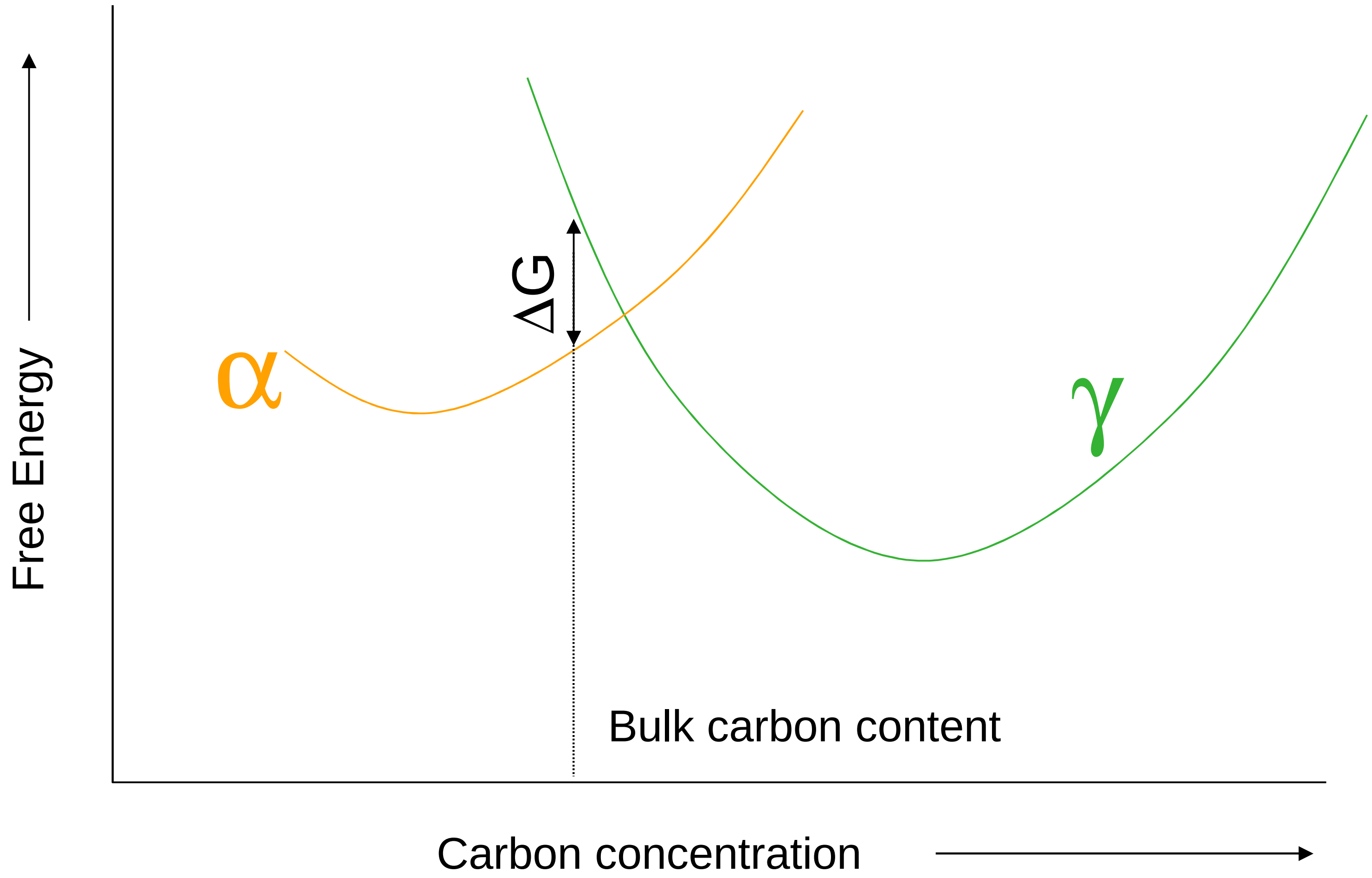


The definition of T_0



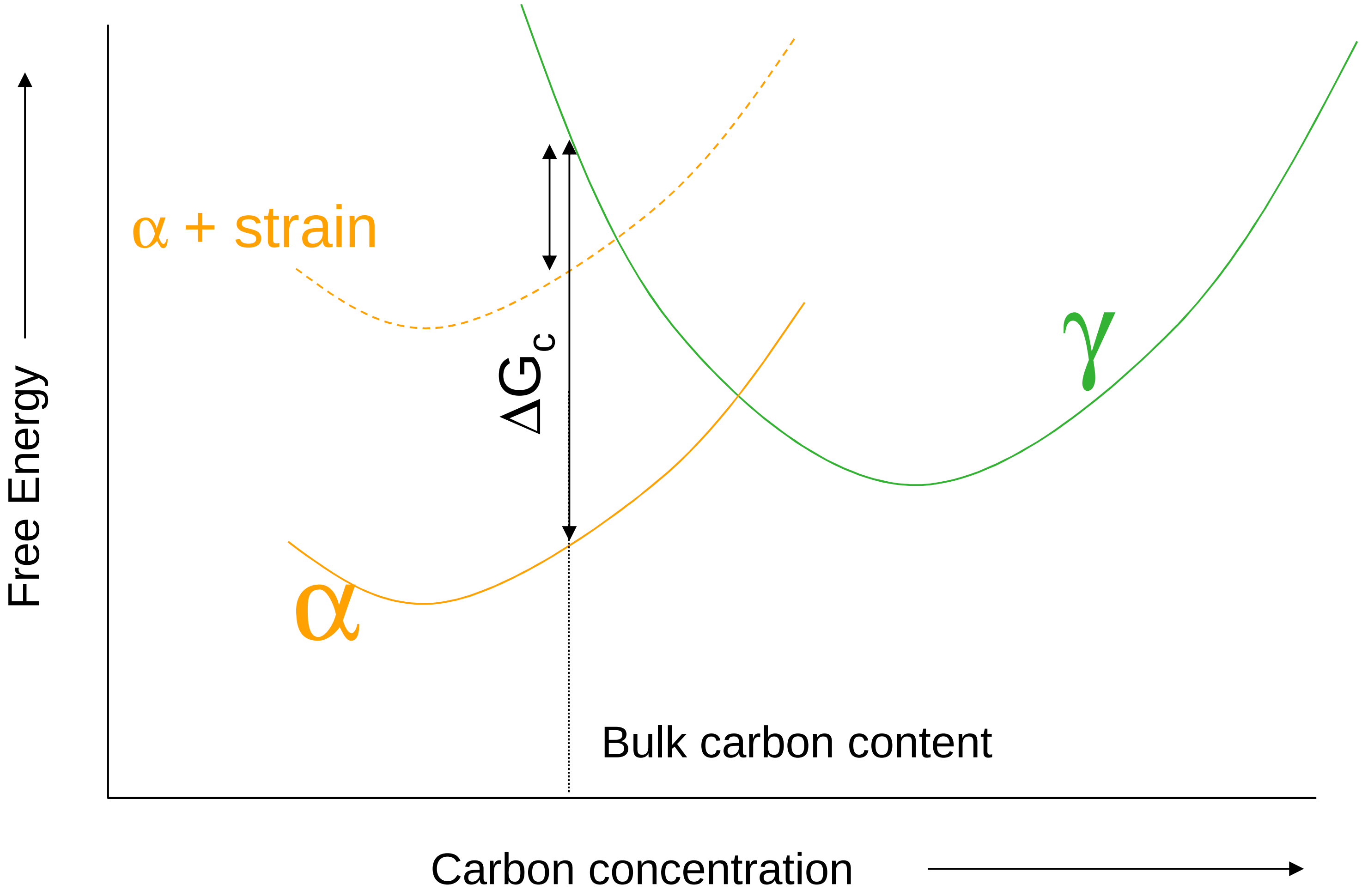
Martensitic transformations require large undercooling below T_0

$$M_s < T < T_0 \quad (\Delta G > 0\text{, but } \Delta G < \Delta G_c)$$



Definition of the critical driving force ΔG_c

$$T = M_s \quad (\Delta G = \Delta G_c)$$



Ghosh and Olson model (1994)

$$\Delta G_{\mathrm{c}} = K_1 + W_\mu (K_\mu^i, x_i)$$

$$\boxed{W_\mu = K_\mu x_{\mathrm{C}}^{0.5} + \sqrt{\sum_j (K_\mu^j x_j^{0.5})^2}}$$

This work:

j = Mn, Si, Cr, Ni or Mo

Modelling approach of Ghosh:

- W_μ : athermal interfacial frictional work
- Specific superposition law (Phythagorean)
- K_μ 's found by model optimization

Modification/improvements:

- Account for Austenite Grain Size effects
- Validate model with M_s data of AHSS/UHSS grades
- Make model calculations without dependence on specific thermodynamic databases

Modified Ghosh model capturing M_s dependence on D^γ

$$\boxed{\Delta G_c = K_1 + W_\mu + {\color{red}W_{HP}} + {\color{green}W_C}}$$

Austenite strengthening, Hall Petch mechanism (Ansell)

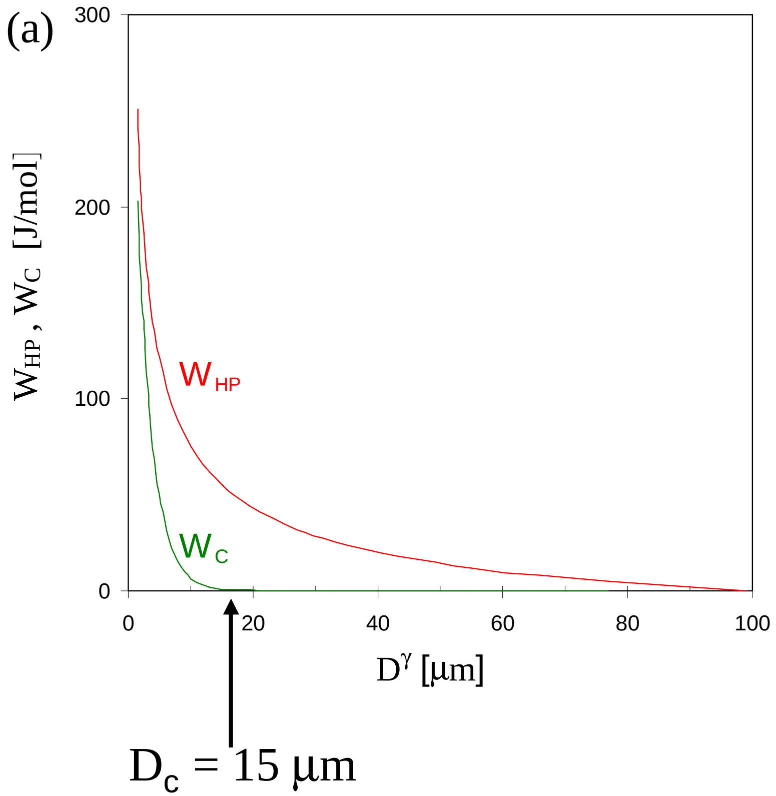
- Higher YS of austenite → more resistance to shape deformation

$$W_{HP} = \frac{K_{HP}}{\sqrt{D^\gamma}}$$

Critical Austenite Grain Size, D_c ~ 15 micron (MPIE/AMMZ)

- Change in aspect ratio laths → change in stored energy (Christian)

$$W_C = K_C \exp\left(-\frac{6D^\gamma}{D_C}\right)$$

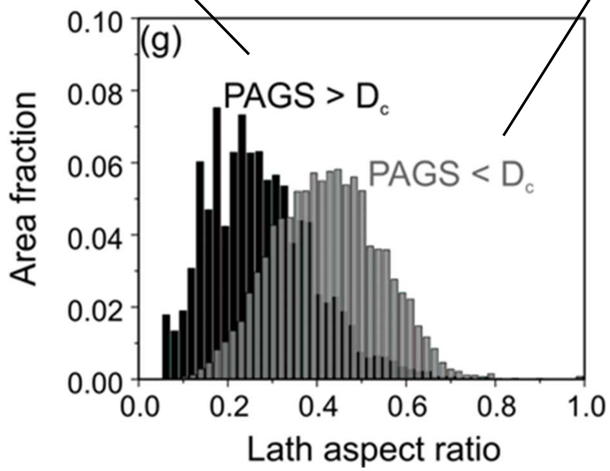


Observations of lath aspect ratio (c/a)

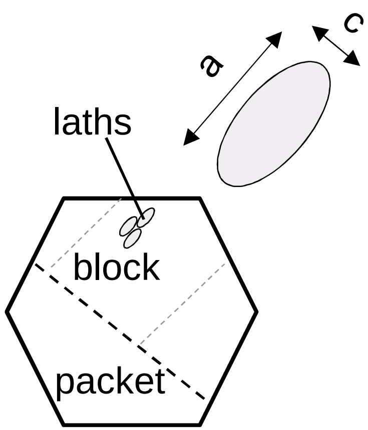
Lutz Morsdorf:
(MPIE)

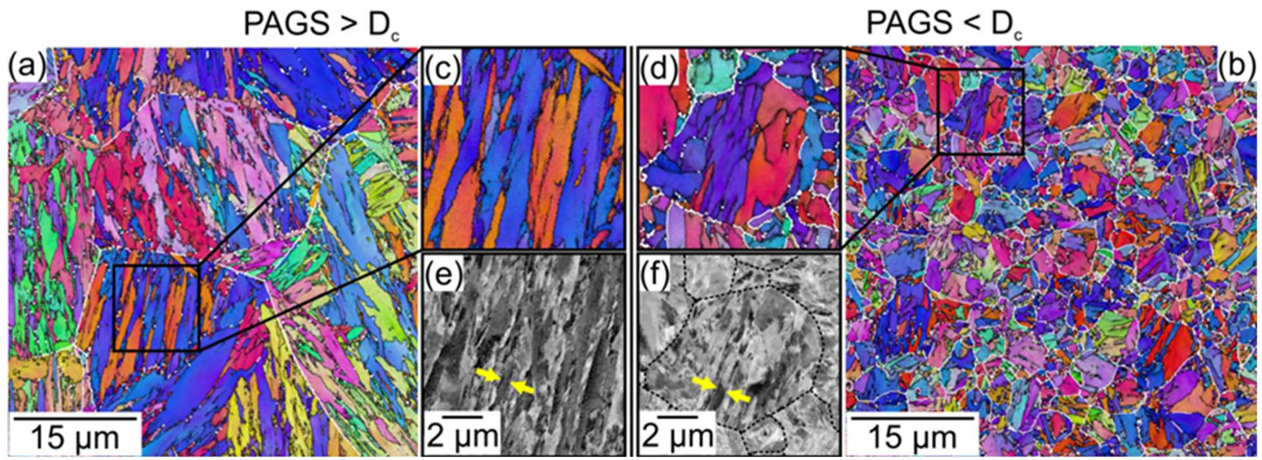
Base alloy: coarse grains

Base + Nb alloy: small grains



- **Length of packets is constrained by small PAGS.**
- **Lath thickness is ~ 200 nm for both alloys.**





Ghosh model capturing M_s dependence on D^γ

$$\Delta G_c = K_1 + W_\mu + W_{HP} + W_C$$

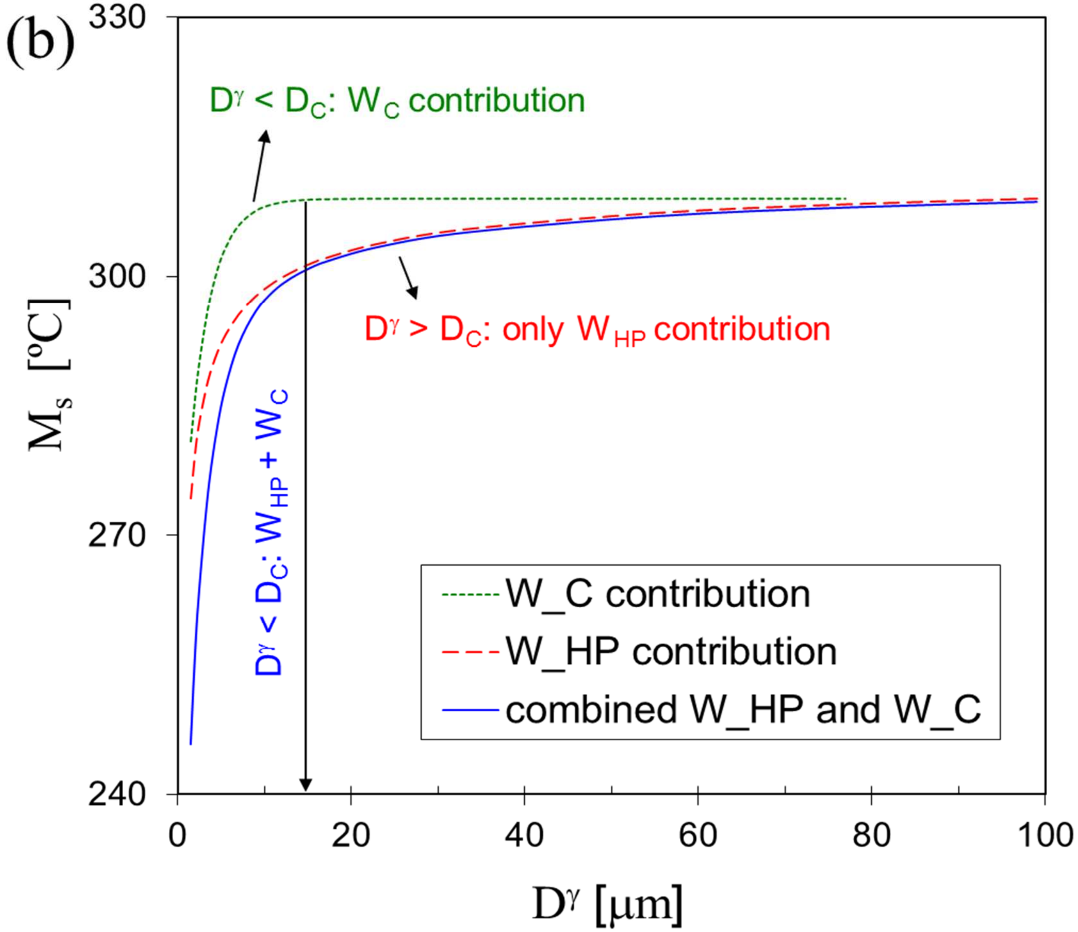
$$W_{HP} = \frac{K_{HP}}{\sqrt{D^\gamma}}$$

K_{HP} = 350 Jμm$^{0.5}$/mol

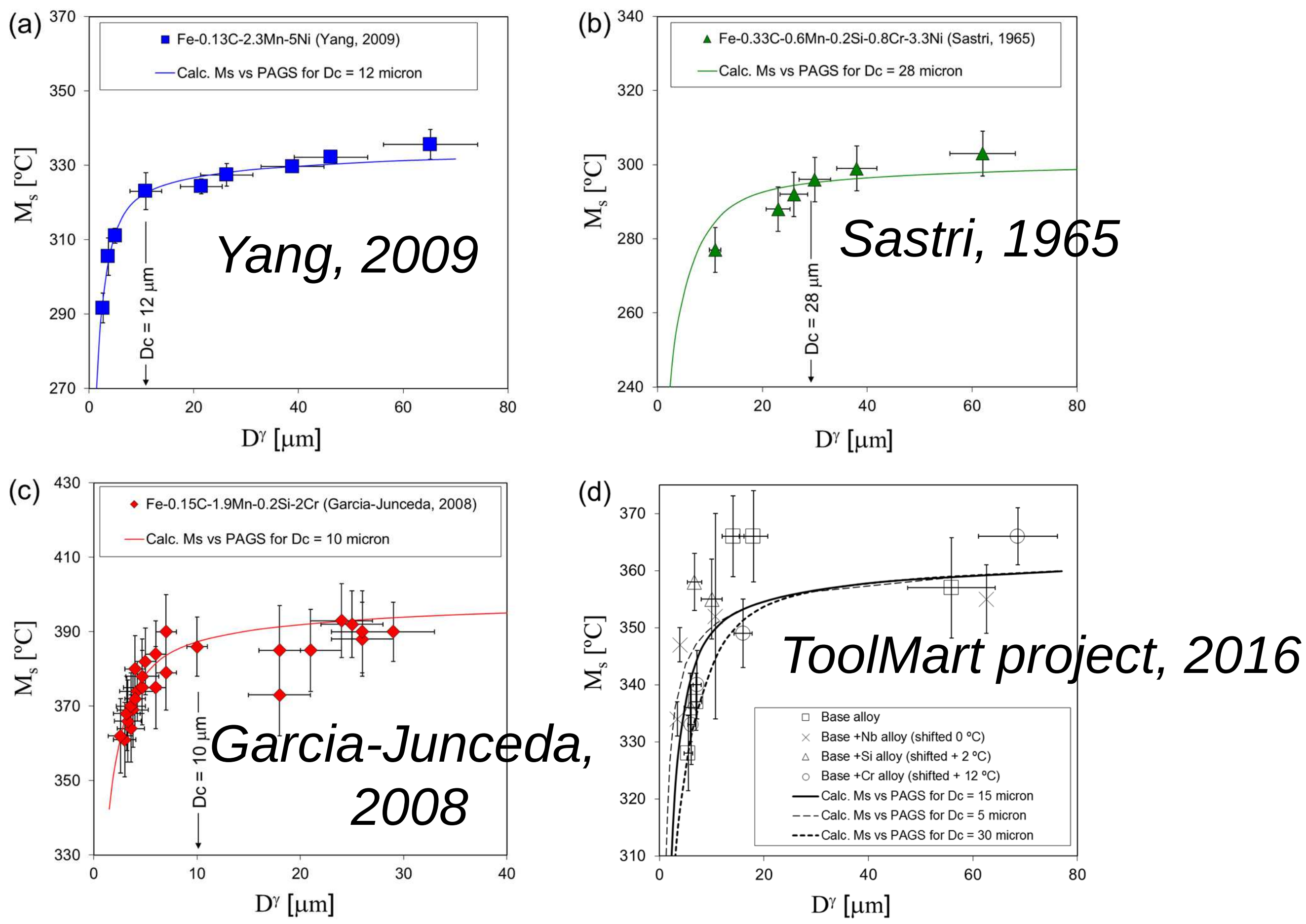
$$W_C = K_C \exp\left(-\frac{6D^\gamma}{D_C}\right)$$

K_C = 370 J/mol

D_C = 15 μm



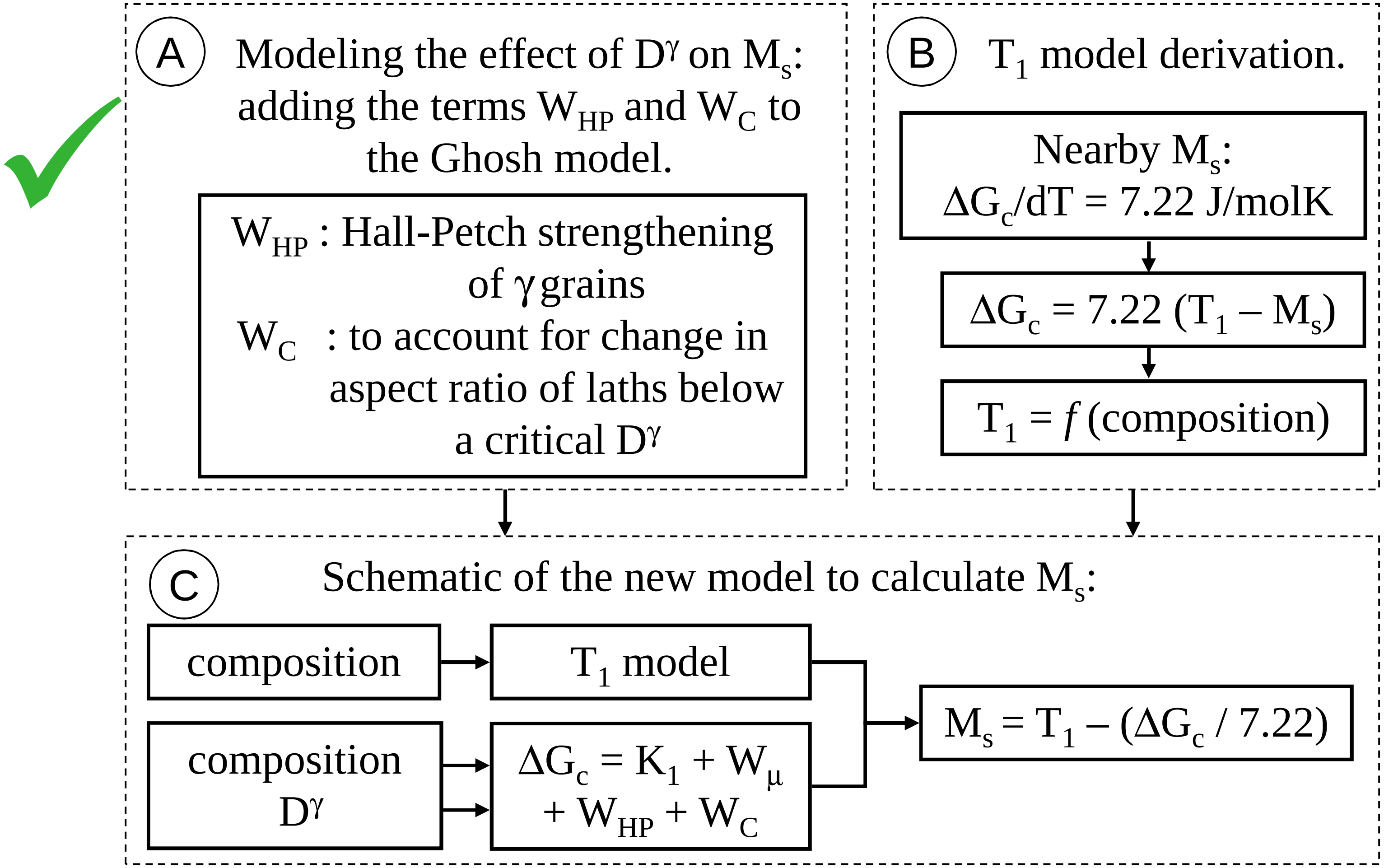
Validation of the model for D^γ effect on M_s



K_C = 370 J/mol, K_{HP} = 350 Jμm$^{0.5}$/mol

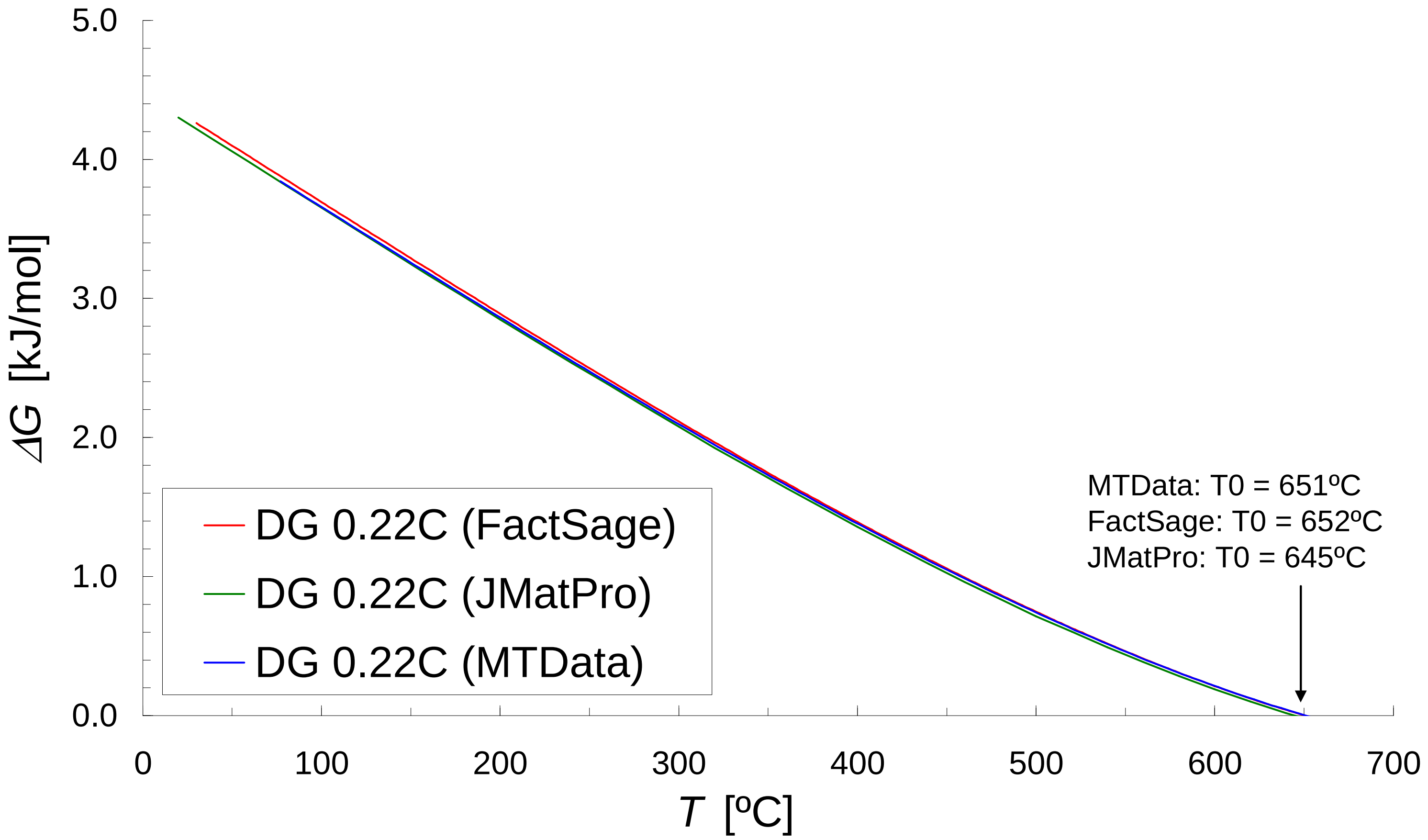
D_C = 10 - 20 µm for most alloys

Schematic of the modeling approach

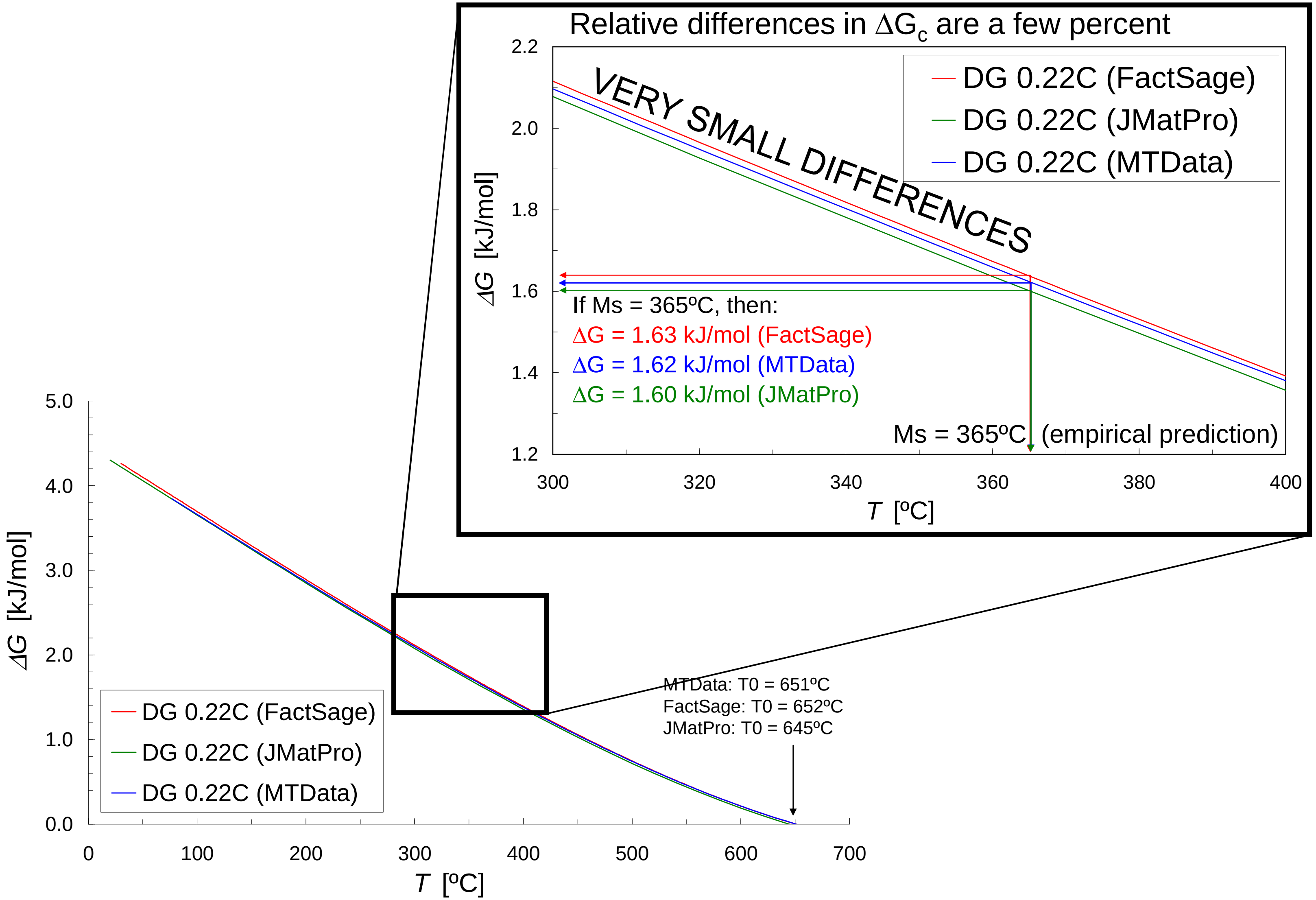


Calculations for Base alloy (0.22C-2.5Mn-0.2Cr-0.2Si)

Comparison of FactSage, MTData & JMatPro

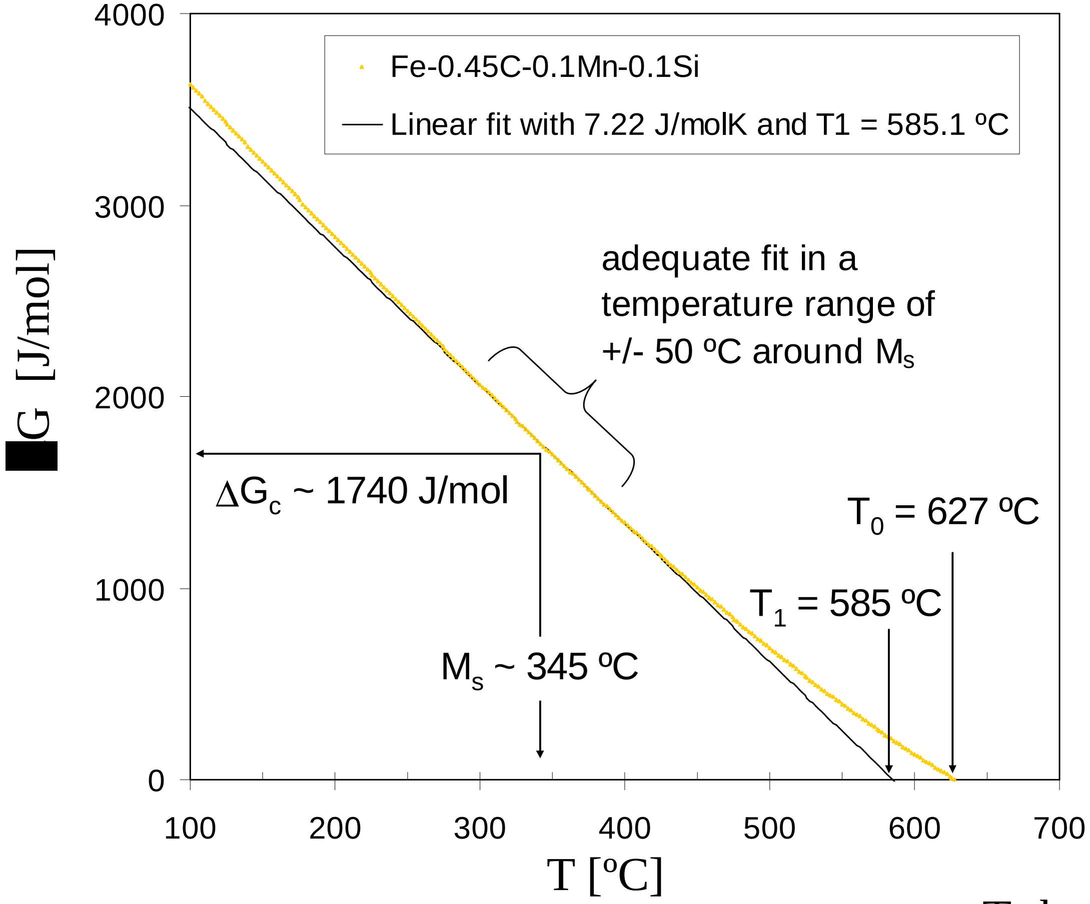


Calculations for Base alloy (0.22C-2.5Mn-0.2Si-0.2Cr)



Linear approximation of ΔG curves is valid nearby Ms

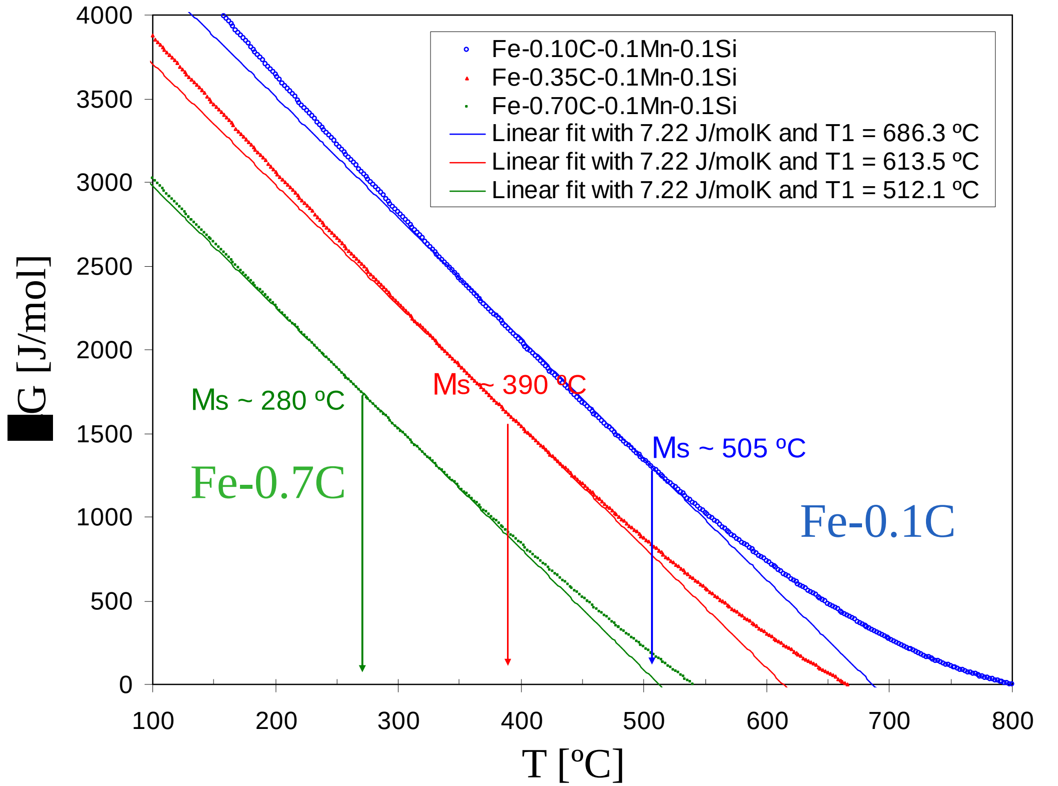
Calculations of ΔG were performed with FactSage



$$\boxed{\Delta G_c = 7.22\,(T_1 - M_s)}$$

T_1 has no physical meaning, it is a mathematical parameter

Linear approximation of ΔG curves

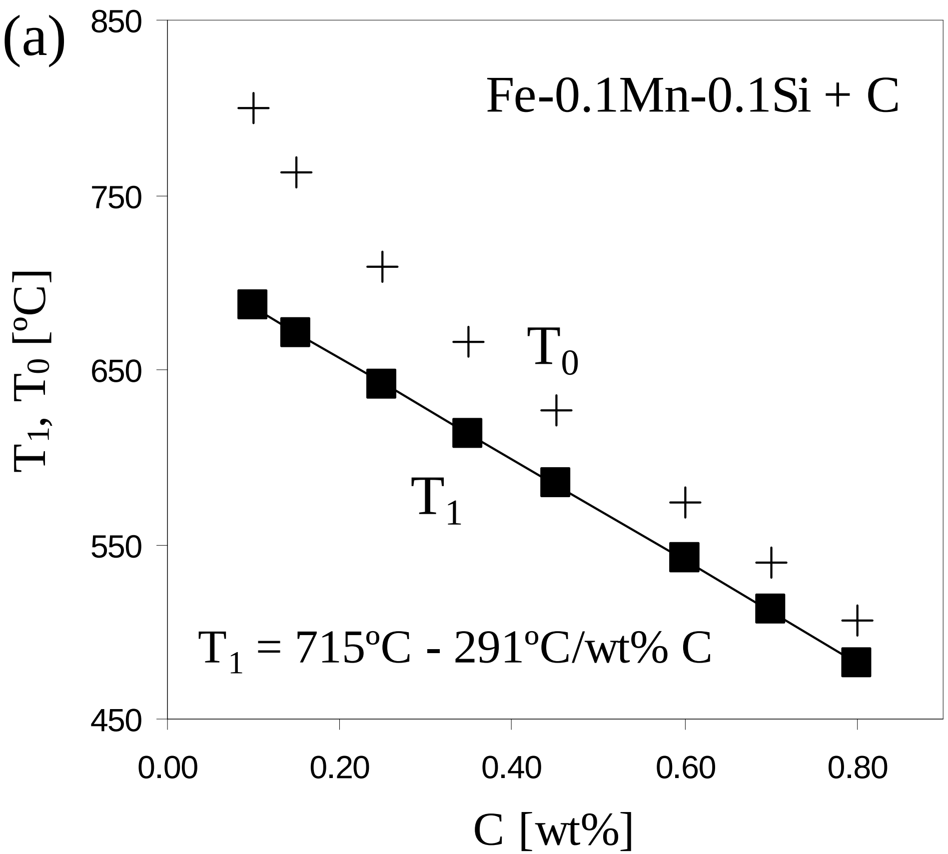


- The linear dependence with slope of 7.22 J/molK seems valid for Fe-C alloys in general.
- A rigorous investigation was started to
  1. Confirm that linearity with a slope of 7.22 J/molK is applicable for all steels
  2. Correlate T_1 temperatures to the chemical composition of steels

T_1 temperatures against C content

Determined with FactSage for plain carbon steels with **0.1Mn and 0.1Si**

(a)

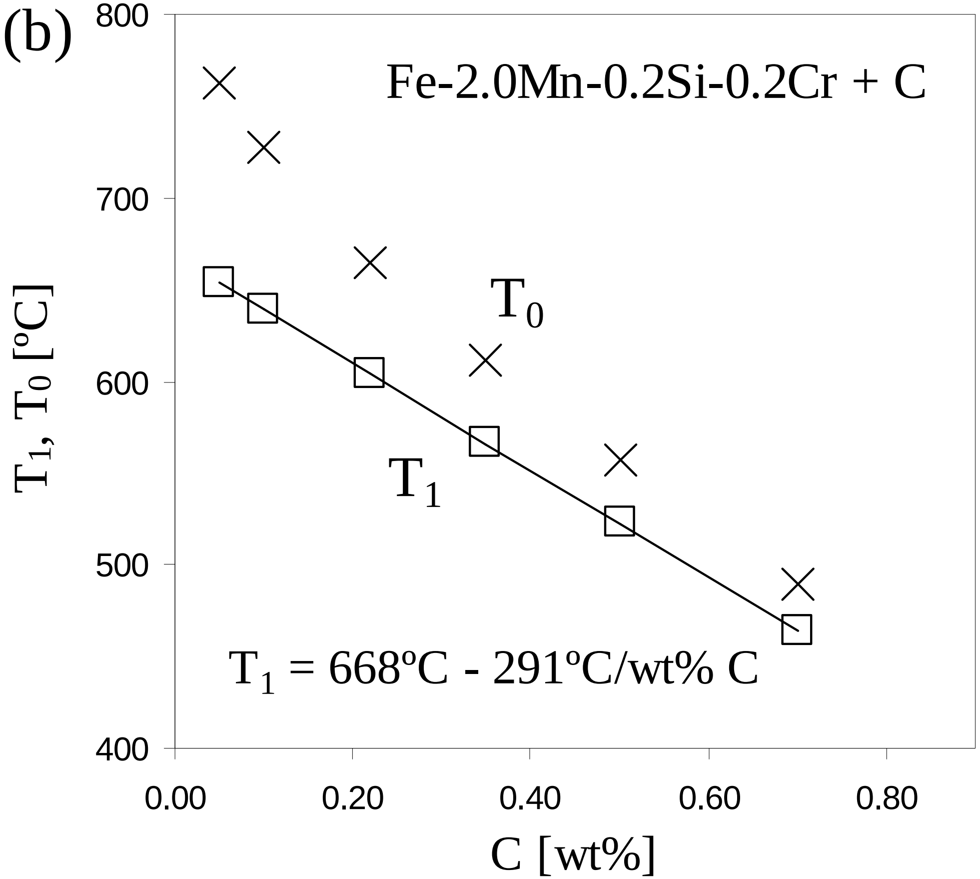


$$T_1 = 715 - 291C$$

T_1 temperatures against C content

Determined with FactSage for alloys with **2.0Mn, 0.2Si and 0.2Cr**

(b)

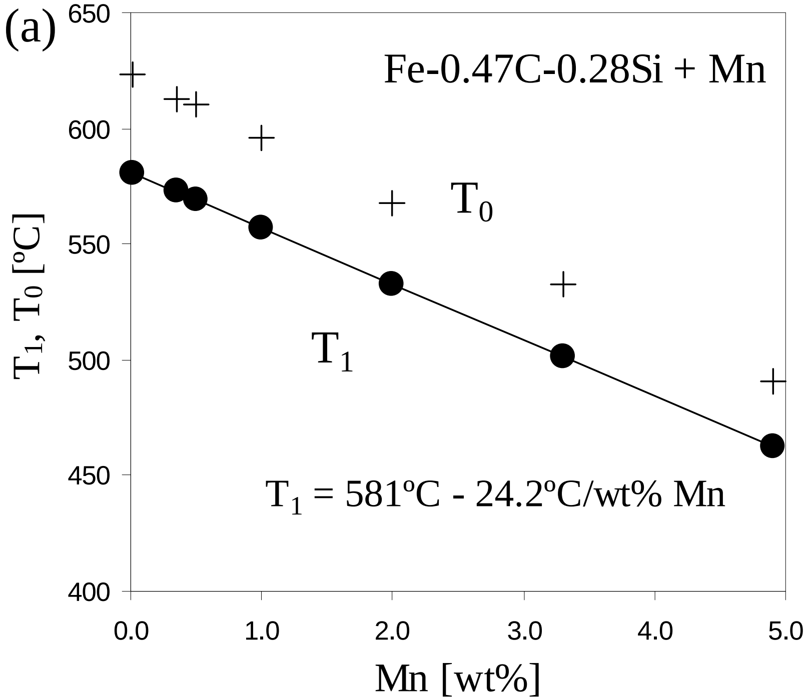


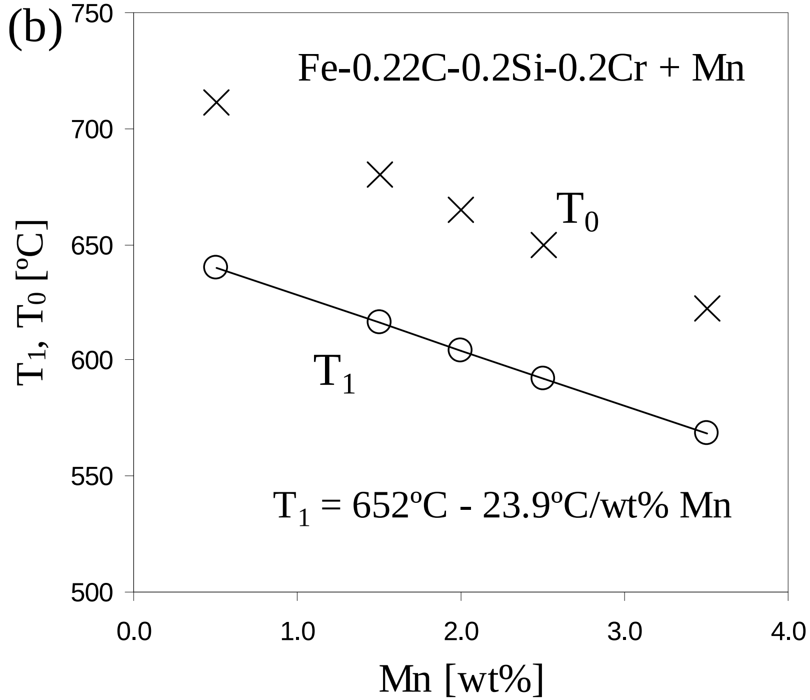
$$T_1 = 668 - \underline{291}C$$

- T_1 dependency on Carbon is not affected by other alloying

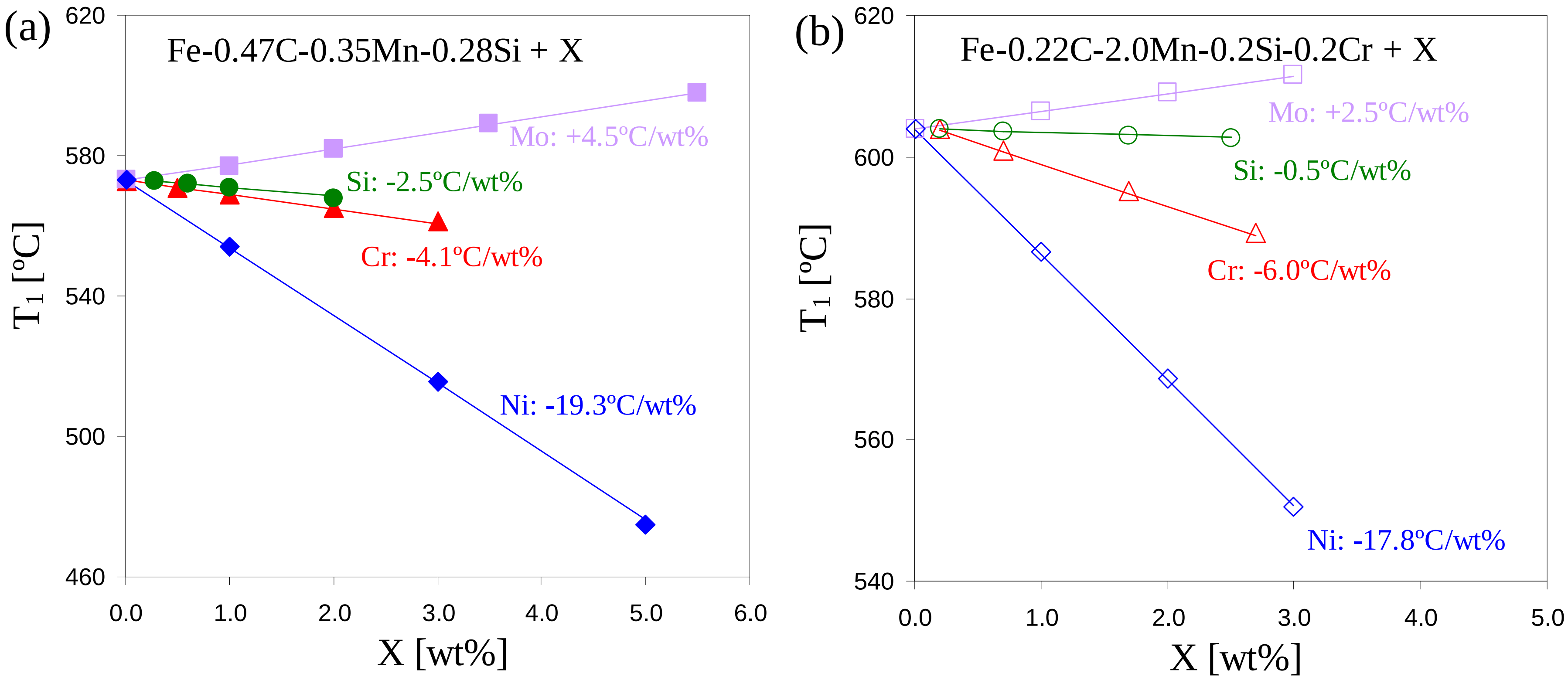
T_1 temperatures against Mn content

$$T_1 = \text{Constant} - \underline{24\text{Mn}}$$





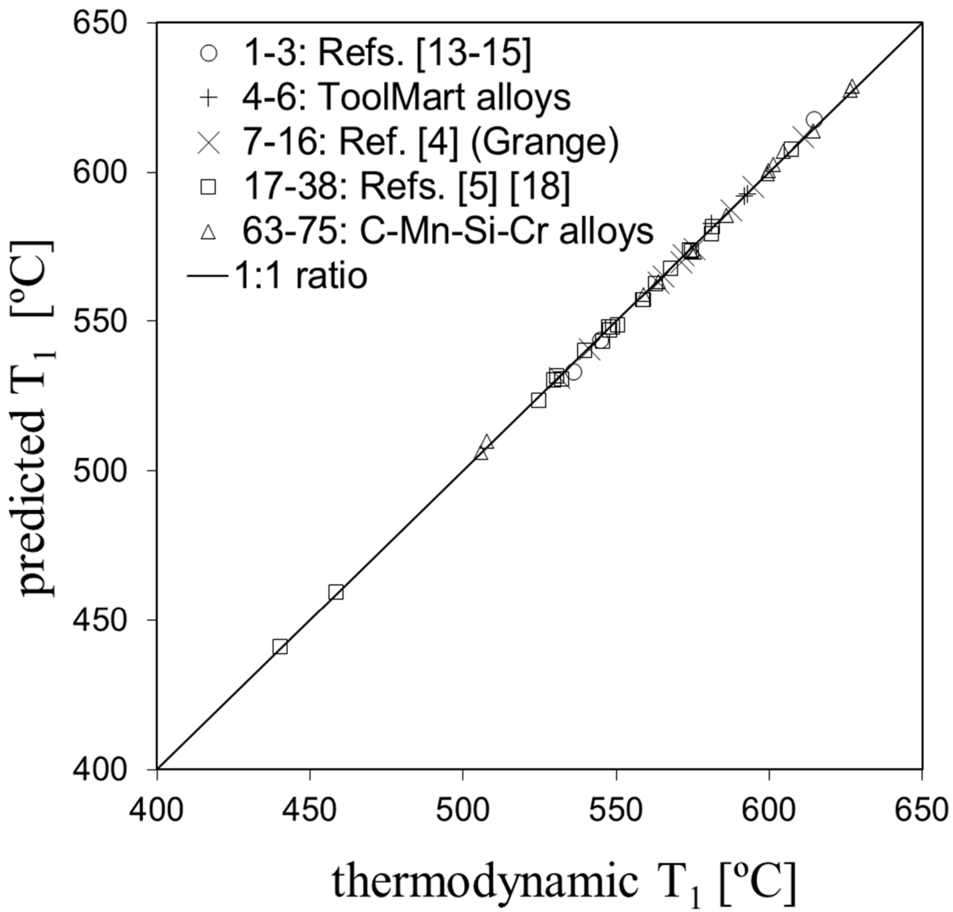
T_1 temperatures against Si, Cr, Ni and Mo contents



$$T_1 = 718 - 291C - 24Mn - 1.5Si - 5.0Cr - 18.5Ni + 3.5Mo$$

Validation T_1 equation with literature data

$$T_1 = 718.3 - 291x_{\mathrm{C}} - 24x_{\mathrm{Mn}} - 1.8x_{\mathrm{Si}} - 5.6x_{\mathrm{Cr}} - 18.4x_{\mathrm{Ni}} + 3.5x_{\mathrm{Mo}}$$



T_1 model benchmarked against FactSage results of **> 70 alloys**:

- Largest deviations ~ 3 ºC
- σ ≈ 1.2 ºC

Schematic of the modeling approach

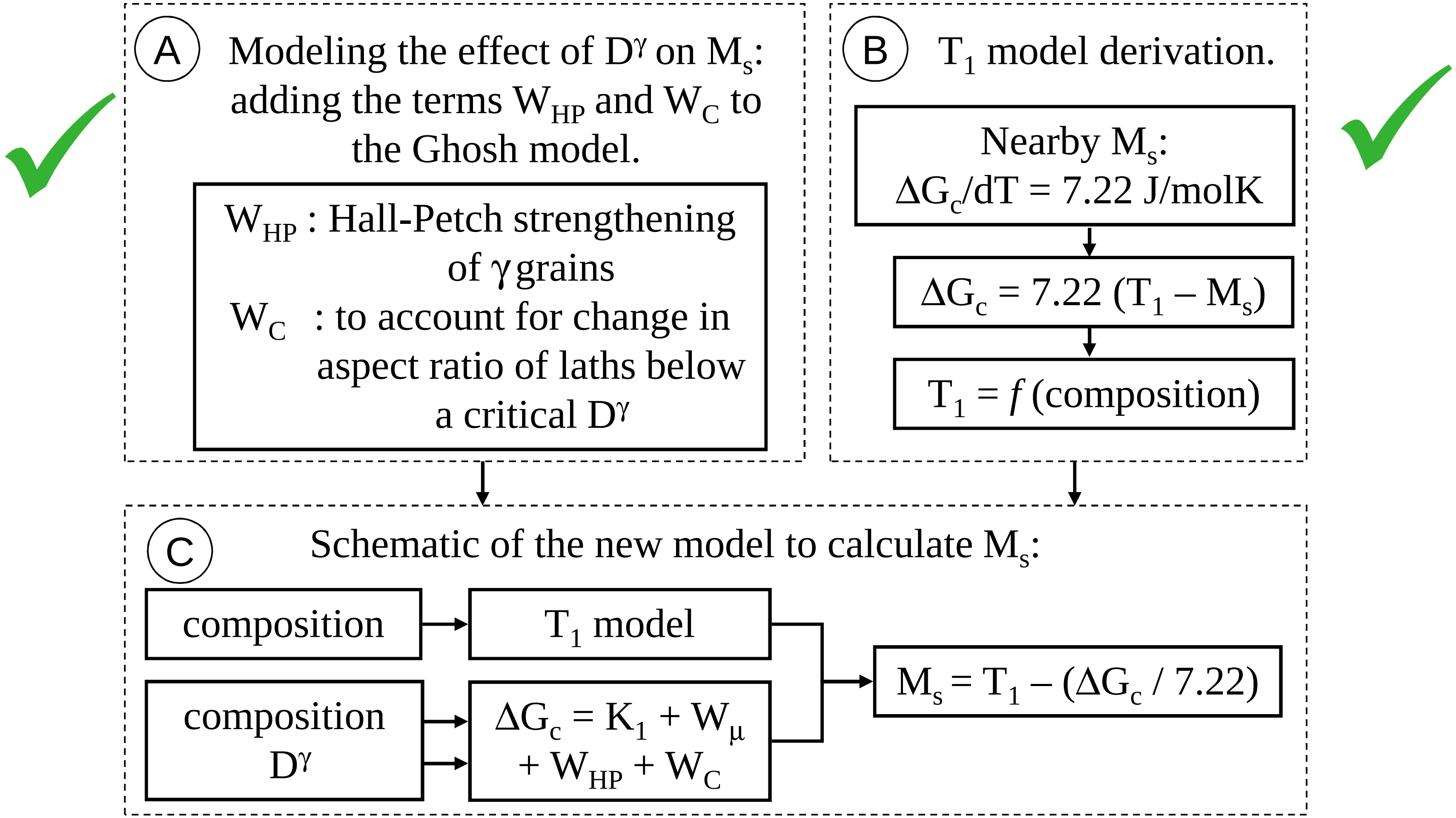


Table 1. Data of alloys used for the validation of the models for T_1, D^{γ} (G) and M_s.

no.	Ref.	grade	C wt%	Mn wt%	Si wt%	Cr wt%	Ni wt%	Mo wt%	exp. G	calc. G	T_1 °C	calc. T_1 °C	exp. M_s °C	calc. M_s °C
1	[16]	Sastri	0.33	0.57	0.23	0.85	3.26	0.09	7.2	6.3	545.0	543.7	298	310
2	[14]	Yang	0.13	2.3			5		7.6	7.4	536.2	533.3	325	308
3	[15]	Garcia	0.15	1.9	0.2	2			7.6	6.5	614.8	617.5	392	382
4		Base	0.22									592.8	337	343
5		Base+Cr	0.22									582.7	328	325
6		Base+Si	0.22									591.9	356	339
7	[4]	SAE-2340	0.37	0.68	0.21		3.41		7.5	8.3	531.6	531.2	305	300
8	[4]	SAE-3140	0.38	0.72	0.21	0.49	1.32		7.5	6.9	564.0	563.0	332	327
9	[4]	SAE-4130	0.29	0							11.3	611.8	377	376
10	[4]	SAE-4140	0.37	0							87.8	587.1	338	346
11	[4]	SAE-4340	0.42	0							41.2	540.7	288	295
12	[4]	SAE-4640	0.36	0							65.4	565.0	338	333
13	[4]	SAE-5140	0.42	[illegible]	[illegible]	[illegible]			[illegible]	[illegible]	[illegible]	574.3	332	334
14	[4]	SAE-6140	0.43	0.74	0.23	0.92			8	7.1	571.2	569.8	327	325
15	[4]	NE-8630	0.30	0.91	0.31	0.52	0.61	0.17	9.5	6.9	594.9	595.1	366	356
16	[4]	NE-9442	0.38	1.08	0.70	0.40	0.34	0.11	10.5	7.6	572.1	572.4	327	321
17	[18] p.96	En16 (6)	0.33	1.48	0.18	0.16	0.26	0.27	7.5	7.6	581.5	581.7	340	340
18	[18] p.96	En17 (7)	0.38	1.49	0.25	0.14	0.24	0.41	8	8.1	567.7	567.7	320	320
19	[5]	En18 (8)	0.39	0.89	0.16	0.88	0.25		5.5	6.6	574.7	573.6	320	335
20	[18] p.96	En18 (9)	0.48	0.86	0.25	0.98	0.18	0.04	5.5	6.9	550.6	548.9	300	302
21	[5]	En19 (10)	0.41	0.64	0.31	1.24	0.18	0.38	8.5	7.9	574.1	574.1	320	325
22	[18] p.98	En19 (11)	0.41	0.67	0.23	1.01	0.20	0.23	8.5	7.2	574.0	574.0	330	328
23	[18] p.98	En21 (12)	0.33	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	540.2	310	309
24	[18] p.101	En24 (17)	0.38	0							58.7	557.3	320	315
25	[18] p.100	En25 (19)	0.31	0							62.9	562.9	320	327
26	[5]	En26 (20)	0.38	0							48.0	546.9	305	307
27	[18] p.101	En26 (21)	0.42	0							29.5	530.5	290	285
28	[18] p.100	En30B (26)	0.32	0.47	0.29	1.21	4.13	0.30	7	9.5	530.5	531.7	295	294
29	[18] p.99	En40B (27)	0.26	0.55	0.21	3.34	0.25	0.54	7.5	9.5	607.1	607.6	360	361
30	[18] p.101	En100 (30)	0.40	1.34	0.21	0.53	1.03	0.22	6	8.0	549.0	548.2	290	303
31	[5]	En110 (32)	0.44	0.58	0.23	1.26	1.40	0.11	7.5	7.4	545.7	543.5	300	297
32	[18] p.100	En110 (33)	0.39	0.62	0.23	1.11	1.44	0.18	7.5	7.8	559.0	557.4	320	315
33	[18] p.100	En23 (35)	0.32	0.61	0.28	0.63	3.22	0.22	7	8.2	547.6	548.0	310	314
34	[18] p.109	En39B (45)	0.15	0.38	0.20	1.16	4.33	0.17	7	7.6	581.0	579.6	365	362
35	[18] p.110	En39B (0.6C)	0.56	0.47	0.18	1.16	4.25	0.18	8	8.1	458.4	459.7	195	206
36	[18] p.96	En45	0.55	0.87	1.74	0.10	0.16	0.02	7.5	6.5	532.1	530.8	260	273
37	[18] p.96	En11	0.59	0.66	0.34	0.65	0.17	0.02	8	6.9	524.8	523.5	280	271
38	[18] p.106	En36 (0.70C)	0.70	0.35	0.16	0.96	3.24	0.06	8.5	7.3	440.1	441.1	185	183
39	[18] p.380	1-3/4 Mn	0.30	1.80	0.15				7	7.1		587.5	350	350
40	[18] p.381	1-1/2 Mn	0.36	1.50	0.20				7.5	7.0		577.2	330	337
41	[18] p.382	1-3/4 Mn	0.38	1.80	0.25				7	7.3		564.1	325	320
42	[18] p.382	1-3/4 Mn	0.46	1.80	0.15				6.5	7.5		541.0	295	292
43	[18] p.384	1-3/4 Si Mn	0.40	0.85	1.75				9	6.8		578.4	340	329
44	[18] p.385	2 Si Mn	0.54	0.85	1.90	0.10	0.16	0.02	7.5	7.3		533.9	285	276
45	[18] p.385	2 Si Mn	0.59	0.85	1.90				7	7.1		522.8	260	263
46	[18] p.387	1 Ni	0.43	0.80	0.20		0.85		7.5	6.4		558.0	335	321
47	[18] p.388	3 Ni	0.30	0.51	0.32	0.07	3.03		7.5	6.8		562.0	340	338
48	[18] p.389	3-1/2 Ni	0.33									540.2	315	309
49	[18] p.390	3-1/2 Ni	0.40									522.1	280	284
50	[18] p.394	1/2 Cr	0.46									564.4	310	321
51	[18] p.394	1 Cr	0.39									581.8	335	340
52	[18] p.395	1/2 Cr	0.59									524.4	260	273
53	[18] p.403	1-1/2 Mn Mo	0.27									603.2	370	366
54	[18] p.403	1-1/2 Mn Mo	0.30									594.4	355	356
55	[18] p.404	1-1/2 Mn Mo	0.32	1.50	0.18			0.27	7.5	7.8		589.8	350	350
56	[18] p.404	1-1/2 Mn Mo	0.35	1.55	0.20			0.28	7.5	8.0		579.9	335	337
57	[18] p.405	1-1/2 Mn Mo	0.37	1.50	0.18			0.27	8	7.9		575.3	330	331
58	[18] p.405	1-1/2 Mn Mo	0.38	1.50	0.25			0.45	8	8.5		572.8	330	326
59	[18] p.443	4 Ni Cr Mo	0.15	0.40	0.25	1.15	4.10	0.20	8	9.3		583.4	365	364
60	[18] p.443	4 Ni Cr Mo	0.30	0.60	0.25	1.25	4.10	0.30	7	10.2		534.8	300	298
61	[18] p.443	4 Ni Cr Mo	0.34	0.50	0.20	1.80	4.00	0.35	9	10.0		524.5	275	278

ToolMart (2016)

Grange (1946)

Steven (1956)

TTT diagrams ASM (1991)

Table 2. Data of 62–121 alloys used for the validation of the M_s model.

no.	Ref.	grade	C wt%	Mn wt%	Si wt%	Cr wt%	Ni wt%	Mo wt%	T_{aus} °C	t_{aus} min.	calc. G	calc. T_1 °C	exp. M_s °C	calc. M_s °C
62	[20]		0.46	0.71	0.26	0.16	0.14		880	2	7.2	563	315	324
63	[20]		0.66	0.69	0.30	0.17	0.10		880	2	7.4	506	265	254
64			0.13	2.00	0.25	0.55			880	2	9.1	629	400	399
65			0.17	1.70	0.40				880	2	8.3	627	400	400
66			0.21	1.70	1.50				920	2	8.8	614	380	376
67			0.22	2.00	0.10	0.61			860	2	9.6	603	365	362
68			0.21	2.00	1.27				900	2	9.4	607	370	367
69			0.20	3.50	1.50				950	2	10.5	573	325	319
70	[21]		0.29	2.39	1.76				950	3	9.2	573	325	321
71			0.31	1.66	1.47				900	3	9.0	586	335	339
72			0.40	1.67	1.48				900	3	9.1	559	300	305
73			0.58	1.54	1.42				900	3	9.0	510	240	246
74									950	2	6.9	601	360	367
75									950	2	7.5	600	360	363
76									950	2	8.0	598	355	358
77									950	2	8.6	597	350	354
78									880	2	9.5	599	365	358
79									880	2	9.6	602	370	361
80									880	2	9.6	605	375	365
81			0.25	2.25	1.15				880	2	10.1	589	340	342
82			0.19	1.97	0.20	0.59			900	4	8.2	612	380	378
83			0.19	2.17	0.20	0.60			900	4	8.5	607	370	370
84			0.19	1.59	0.20	0.81			900	4	7.9	620	380	388
85			0.19	1.79	0.20	0.77			900	4	8.1	615	375	381
86			0.19	2.16	0.20				900	4	7.7	611	380	379
87			0.19	1.99	0.20	0.30			900	4	7.9	613	380	381
88			0.19	2.05	0.07	0.60			900	4	8.1	610	380	376
89			0.20	2.04	0.19	0.60			900	4	8.3	609	380	373
90	[1]	1Mn	0.47	1.02	0.34				982	10	4.3	556	310	317
91	[1]	3Mn	0.47	3.33	0.26				982	10	7.3	501	230	238
92	[1]	5Mn	0.44	4.87	0.29				982	10	9.3	473	188	197
93	[1]	1Si	0.47	0.40	1.06				982	15	4.1	570	321	334
94	[1]	1Ni	0.45	0.36	0.31		1.16		927	30	4.0	557	310	329
95	[1]	3Ni	0.46	0.34	0.28		3.36		927	30	4.6	514	282	286
96	[1]	5Ni	0.46	0.35	0.30		4.83		927	30	5.0	487	257	258
97	[1]	1Cr	0.50	0.32	0.27	0.98			1260	3	1.2	559	313	320
98	[1]	1Mo	0.50							3	2.5	568	330	323
99	[1]	3Mo	0.49							3	7.5	580	305	308
100	[1]	3Ni-1Cr	0.46							5	3.1	509	260	272
101	[1]	1Mn	0.47	[illegible]	[illegible]				[illegible]	30	5.8	556	310	316
102	[1]	1Mn	0.47	1.02	0.34				982	10	4.3	556	310	317
103	[1]	1Mn	0.47	1.02	0.34				1093	10	2.5	556	313	319
104	[1]	3Ni	0.46	0.34	0.28		3.36		927	30	4.6	514	282	286
105	[1]	3Ni	0.46	0.34	0.28		3.36		982	20	3.8	514	282	287
106	[1]	3Ni	0.46	0.34	0.28		3.36		1093	10	2.5	514	280	288
107	[1]	4042	0.43	0.90	0.23	0.27	0.23	0.26	816	10	8.6	566	321	320
108	[1]	4063	0.64	0.85	0.29	0.24	0.19	0.27	816	10	8.9	507	230	248
109	[1]	8442	0.40	1.43	0.22	0.29	0.23	0.32	816	10	9.6	562	316	310
110	[1]	8949	0.49	1.01	0.20	0.56	0.54	0.38	816	10	9.6	539	280	282
111	[1]	8749	0.52	0.85	0.21	0.50	0.53	0.26	816	10	9.0	535	282	280
112	[1]	4142	0.41	0.86	0.30	1.06	0.11	0.23	816	10	9.5	571	310	318
113	[1]	4160	0.61	0.59	0.24	0.94	0.16	0.33	857	10	8.4	519	260	259
114	[1]	4342	0.42	0.68	0.18	0.81	1.74	0.29	816	10	9.5	544	277	295
115	[1]	special	0.30	1.63	0.49	0.44	0.00	0.33	899	10	8.2	590	346	344
116	[19]	B	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	7.4	558	311	323
117	[19]	C	[illegible]								[illegible]	499	246	251
118	[19]	D	[illegible]								[illegible]	444	185	184
119	[19]	5	[illegible]								[illegible]	596	354	359
120	[19]	2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]		[illegible]	[illegible]	[illegible]	534	285	282
121	[19]	6	0.78	0.33	0.02	1.42	0.27		1066	15	3.3	470	210	211

Tata Steel (2008-2016)

Payson (1944)

Rowland (1946)

Validation of the new M_s model

$$\Delta G_c = K_1 + W_\mu + \frac{K_{HP}}{\sqrt{D^\gamma}} + K_C \exp\left(-\frac{6D^\gamma}{D_C}\right)$$

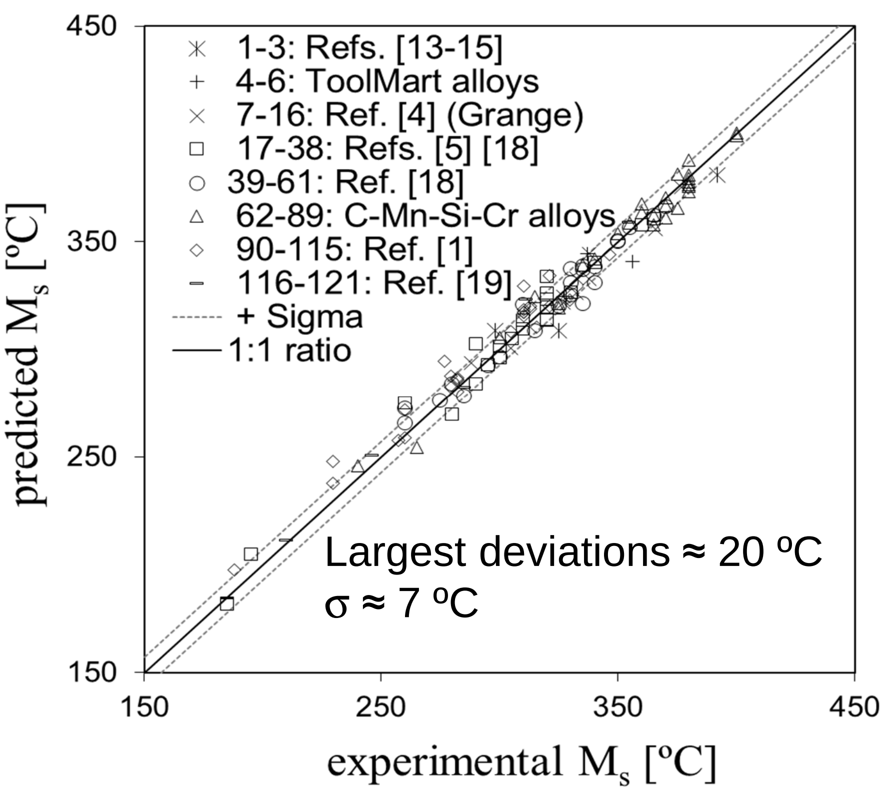
$K_1 = 1015$ J/mol $\quad W_\mu = 670x_C^{0.5} + \sqrt{(195x_{Mn}^{0.5})^2 + (140x_{Si}^{0.5})^2 + (170x_{Cr}^{0.5})^2 + (5x_{Ni}^{0.5})^2 + (205x_{Mo}^{0.5})^2}$

$K_{HP} = 350$ Jμm$^{0.5}$/mol

$K_C = 370$ J/mol

$D_C = 11$ μm

Alloying ranges tested:
0.1 - 0.7 C
0 - 3 Mn
0 - 2 Si
0 - 3 Cr
0 - 5 Ni
0 - 1 Mo



Benckmarking to other models

Table: standard errors associated with different models tested against alloys 1-121

Overall model performance

alloys 90-115: Payson data

Model	σ (ºC)	σ (ºC) evaluated for various datasets (alloy series)						
	1–121	1–6	7–16	17–38	39–61	62–89	90–115	116–121
Payson (1944)	**17**	37	15	22	13	18	**9**	16
Carapella (1944)	**23**	48	14	23	16	31	12	21
Nehrenberg (1946)	**14**	25	6	15	11	12	17	21
Grange (1946)	**19**	35	7	26	16	15	18	20
Steven (1956)	**18**	20	6	15	9	22	18	39
Andrews (1965)	**11**	16	5	10	10	12	10	23
Eldis (1977)	**16**	32	13	16	14	14	16	20
Van Bohemen (2012)	**11**	20	5	7	9	13	10	9
JMatPro 6.1	**14**	19	15	12	10	12	18	7
This work	**7**	13	6	7	6	6	9	6

Thank you for your attention!

Do you have any questions?