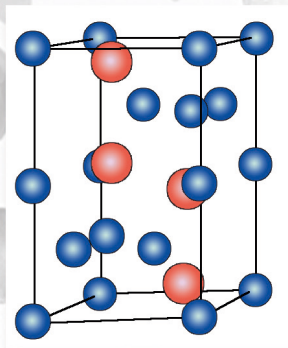


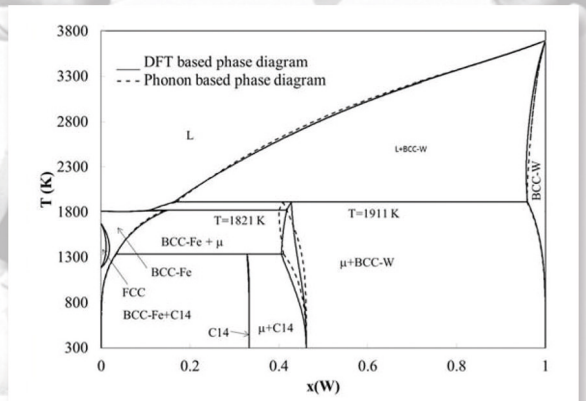
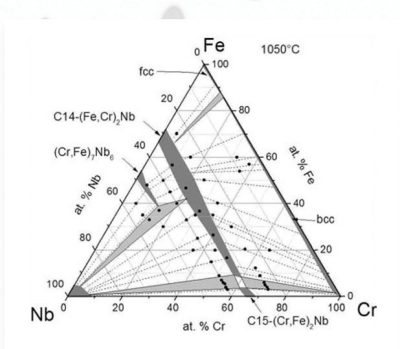
Thermochemical Modeling of Laves Phase Containing Ferritic Steels

Aurélie Jacob

$$\mathcal{H}\psi = \mathcal{H}E$$



$$G = a + bT + cT \ln T + \sum d_n T^n$$



Energie & Umwelt /
Energy & Environment
Band / Volume 274
ISBN 978-3-95806-070-8

Forschungszentrum Jülich GmbH
Institute of Energy and Climate Research (IEK)
Microstructure and Properties of Materials (IEK-2)

Thermochemical Modeling of Laves Phase Containing Ferritic Steels

Aurélie Jacob

Schriften des Forschungszentrums Jülich
Reihe Energie & Umwelt / Energy & Environment

Band / Volume 274

ISSN 1866-1793

ISBN 978-3-95806-070-8

Contents

Introduction.....	1
Scope of the work	3
Chapter I – Contents of the study.....	5
I. Ferritic steel	5
II. Literature survey	7
1. Laves phases	7
2. Silicon in Laves phase	10
3. Thermodynamic stability of Laves phase containing system.....	11
3.1 Cr-Nb	11
3.2 Fe-Nb	13
3.3 Fe-W	16
3.1 Cr-Nb-Si.....	18
3.2 Fe-Nb-Si.....	20
3.3 Cr-Fe-Nb	25
3.4 Fe-W-Si.....	26
3.5 Summary of the literature survey.....	28
Chapter II – Methods	31
I. Introduction.....	31
II. Experimental phase diagram investigations.....	33
III. Calculation of Phase diagrams (Calphad).....	34
1. Introduction.....	34
2. Models for the Gibbs energy.....	35
2.1 Unary phase	36
2.2 The compound energy formalism=sublattice modeling.....	37
3. Input data	40
4. Optimization of parameters in the Gibbs energy models.....	42
4.1 Principle	42
4.2 Modeling of the Gibbs energy	43
4.3 Optimization process in the present work.....	45
IV. Density Functional Theory.....	46
1. Introduction.....	46
2. Born-Oppenheimer approximation	47

3.	The Hohenberg-Kohn theorem	47
4.	The Kohn-Sham approach	48
4.1	The exchange correlation energy	48
4.2	Basis sets	49
4.3	Self-consistency loop	50
5.	Description of the electrons: all-electrons and pseudo-potential methods	50
5.1	All-electrons method	50
5.2	Pseudo-potential methods	50
5.3	The projector augmented wave method (PAW)	51
5.4	Periodicity of the system	51
5.5	Brillouin zone integration	52
6.	DFT calculations in the present work	52
V.	Phonon calculations	53
1.	Theory	53
2.	Thermodynamics	54
2.1	Harmonic approximation	54
2.2	Einstein model	55
2.3	Debye model	56
2.4	Polynomial function	56
3.	Quasi-harmonic approximation	57
4.	Results	58
	Chapter III - Pure elements and binary boundary systems	59
I.	Pure elements	59
1.	Energy of formation	59
2.	Phonon calculations of the pure elements	62
2.1	Iron, Fe	63
2.2	Tungsten, W	66
II.	Binary boundary systems	68
1.	Calculation in binary systems: Fe-Nb, Fe-Si, Nb-Si, Cr-Nb	68
2.	Cr-Nb	71
3.	DFT calculations in other systems	73
	Chapter IV – Modeling of Fe-W phase diagram using first-principles and phonons calculations	74
	Introduction	74

I.	Literature survey	75
II.	Modeling	76
1.	Density Functional Theory (DFT)	76
2.	Density Functional Theory Phonon Calculations	77
3.	Calphad modeling	80
3.1.	Substitutional solutions: Liquid, BCC, FCC.....	81
3.1.	λ -Fe ₂ W C14-Laves phase	81
3.2.	μ -phase.....	82
4.	Optimization method	83
4.1	BCC, Liquid, FCC	83
4.2	FCC.....	85
4.3	The intermetallic phases: Laves- and μ -phases.....	85
III.	Results and discussions.....	87
1.	DFT calculations.....	87
2.	Phonon results	91
3.	Thermodynamic optimization.....	96
3.1.	DFT based phase diagram.....	96
3.2.	Phase diagram based on phonon calculations	99
3.3.	Comparison of the phase diagrams	103
	Conclusion	106
	Chapter V – The Cr-Fe-Nb system	107
	Introduction.....	107
	Literature.....	107
I.	Experimental determination of the isothermal sections at 700°C, 1050°C and 1350°C.....	109
1.	Experimental.....	109
2.	Results and discussion	110
2.1	Extension of C15 and C14 laves phase (Fe,Cr) ₂ Nb in the ternary system.....	113
2.2	The Nb rich side.....	117
2.3	The Cr-Fe side.....	120
	Conclusion	122
II.	Thermal and solidification behavior of the Cr-Fe-Nb system	132
1.	Results.....	133
2.	Discussion	136

2.1	Cr-Nb side.....	136
1.1.	Fe-Nb side.....	138
1.2.	Cr-Fe side.....	138
1.3.	Ternary invariant reaction.....	139
	Conclusion	140
III.	Thermodynamic modeling of the Cr-Fe-Nb ternary system.....	146
1.	Literature review.....	146
1.1.	Fe-Nb	146
1.2.	Fe-Cr.....	146
1.3.	Cr-Nb	147
1.4.	Cr-Fe-Nb.....	147
2.	Thermodynamic modeling.....	148
2.1.	Solution phases: BCC, FCC and Liquid	148
2.2.	σ phase	148
2.3.	Laves phases C14 and C15	149
2.4.	μ phase	150
3.	DFT calculations.....	151
4.	Results and discussions.....	152
4.1	DFT calculations.....	152
4.2	Optimization of the phase diagram	159
4.3	Results of the optimization of the phase diagram	162
	Chapter VI – Thermodynamic modeling of the Fe-Nb-Si system	165
	Introduction.....	165
I.	Literature.....	165
II.	Thermodynamic modeling.....	166
1.	Fe-Nb	167
2.	Nb-Si.....	168
3.	Fe-Si.....	168
4.	Fe-Nb-Si.....	169
4.1	Laves phase.....	169
4.2	μ phase	170
4.3	Ternary compounds	170
III.	DFT calculations.....	171

IV. Results and discussion	172
1. DFT calculations	172
1.1 C14 Laves phase	172
1.2 μ phase	173
1.3 Ternary phases	176
2. Thermodynamic optimization of the phase diagram	176
2.1 Dissolution of Si in the Laves phase	178
2.2 Si in the μ phase	178
2.3 Results of the thermodynamic assessment	178
Conclusion	181
Chapter VII – Microstructure of alloys and phase equilibria of sub-system Laves phase containing systems	182
I. Development of laves phase strengthened ferritic steel	182
II. Development of Nb-silicide	184
III. Phase diagram vs ferritic steel alloy	185
Conclusion	187
Bibliography	189

**Energie & Umwelt /
Energy & Environment
Band / Volume 274
ISBN 978-3-95806-070-8**

