

List of Symbols	i
List of acronyms	iii
List of Tables.....	v
List of Figures	vii
Preface.....	xv
Chapter 1 Introduction	1
1.1 <i>High Entropy Alloys</i>	2
1.2 <i>Criteria and methods for predicting HEA stability</i>	3
The Hume-Rothery Rules	3
Mixing Entropy (ΔS_{mix}).....	4
Mixing Enthalpy (ΔH_{mix})	7
The Delta (δ) parameter.....	7
Computational thermodynamics approach	8
1.3 <i>Development of the Thermodynamic database</i>	9
Phase Diagrams and Thermochemical Data	10
1.4 <i>Thermodynamic Software and Database packages</i>	11
Commercial Softwares.....	11
Databases for HEAs.....	13
1.5 <i>Thermodynamic Models</i>	13
Gibbs energy of pure components	14
Gibbs energy of stoichiometric phases	15
Gibbs energy of solutions	15
Models for treating SROs in solutions.....	17
1.6 <i>Cluster Expansion–Cluster Variation Methods (CE–CVM)</i>	18
Configurational variables.....	18

Cluster expansion method.....	21
Cluster variation method.....	23
1.7 <i>First-principles approaches to disordered alloys</i>	25
SQS	27
1.8 <i>Scope of the present investigation</i>	28
Chapter 2 Computational Methodology.....	31
2.1 <i>Introduction</i>	31
2.2 <i>DFT calculations</i>	31
2.3 <i>Cluster Expansion</i>	33
2.4 <i>Generation of special quasi-random structures</i>	34
2.5 <i>Thermodynamic Assessment</i>	36
Simultaneous optimization.....	37
2.6 <i>Calculation of thermodynamic quantities</i>	37
2.7 <i>Evaluation of Warren Cowley parameters</i>	38
Chapter 3 First-Principles Calculations	41
3.1 <i>Introduction</i>	41
3.2 <i>Nb-Ti System</i>	41
3.3 <i>Ti-V System</i>	45
3.4 <i>Ti-Zr System</i>	49
3.5 <i>Nb-V System</i>	53
3.6 <i>Nb-Zr System</i>	57
3.7 <i>V-Zr System</i>	61

3.8	<i>Nb-Ti-V System</i>	65
3.9	<i>Nb-Ti-Zr System</i>	69
3.10	<i>Nb-V-Zr System</i>	73
3.11	<i>Ti-V-Zr System</i>	77
3.12	<i>Nb-Ti-V-Zr system</i>	81
	Comparative study of CECs of the binary ternary and quaternary system.....	85
3.13	<i>Conclusions</i>	87
Chapter 4 Thermodynamic Description of the bcc Nb-Ti-V-Zr System.....		89
4.1	<i>Introduction</i>	89
4.2	<i>Nb-Ti System</i>	89
4.3	<i>Ti-V system</i>	94
4.4	<i>Ti-Zr system</i>	98
4.5	<i>Nb-V system</i>	104
4.6	<i>Nb-Zr system</i>	110
4.7	<i>V-Zr system</i>	116
4.8	<i>Transformation of parameters from orthogonal basis to CV basis</i>	119
4.9	<i>Thermodynamic description of bcc Nb-Ti-V-Zr System</i>	120
4.10	<i>Conclusions</i>	121
Chapter 5 Thermodynamic Calculations of bcc Nb-Ti-V-Zr System		123
5.1	<i>Introduction</i>	123
5.2	<i>Binary Systems</i>	123
5.3	<i>Ternary systems</i>	127

5.4	<i>Quaternary System</i>	134
5.5	<i>Effect of temperature on entropy</i>	138
5.6	<i>Effect of pure ternary CECs on thermodynamic quantities</i>	139
5.7	<i>Conclusions</i>	140
Chapter 6 Short-Range Ordering in bcc Nb-Ti-V-Zr System		143
6.1	<i>Introduction</i>	143
6.2	<i>Binary systems</i>	143
6.3	<i>Ternary systems</i>	145
6.4	<i>Quaternary system</i>	155
6.5	<i>Effect of pure ternary CEC on SROs</i>	157
6.6	<i>Conclusions</i>	158
Chapter 7 Summary And Suggestions For Future Work.....		159
References.....		161
Appendix A.....		185
Appendix B.....		193
Appendix C.....		197
Appendix D.....		199
Appendix E		201
List of Research Papers.....		203