

*Short-range order in high entropy alloys:
Thermodynamic modeling and application to
Nb-Ti-V-Zr system*

Thesis submitted for the degree of

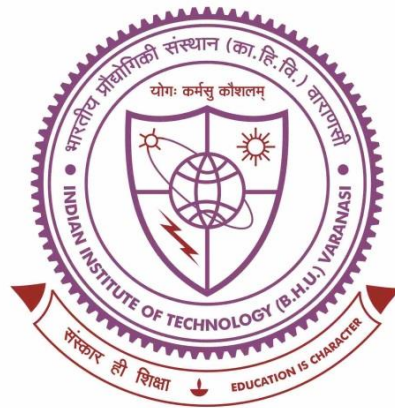
Doctor of Philosophy

in

Metallurgical Engineering

by

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2023

CERTIFICATE

It is certified that the work contained in the thesis titled “*Short-range order in high entropy alloys: Thermodynamic modeling and application to Nb-Ti-V-Zr system*” by *Shanker Kumar* has been carried out under my supervision and this work has not been submitted elsewhere for a degree.

It is further certified that the student has fulfilled all the requirements of Comprehensive, Candidacy and SOTA for the award of Ph.D. degree.



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DECLARATION BY THE CANDIDATE

I, **Shanker Kumar**, certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of **Dr. Vikas Jindal** from **July 2017** to **May 2023**, at the **Department of Metallurgical Engineering**, Indian Institute of Technology (BHU), Varanasi. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc.*, reported in journals, books, magazines, reports, dissertations, theses, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.

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LIST OF SYMBOLS

α_i	Cowley–Warren SRO parameter for i^{th} neighbor pairs
ϕ	thermodynamic potential
γ_i	Kikuchi–Barker coefficient for cluster i
ρ_i	the cluster variable for cluster i
σ_i	site operator
G^φ	total Gibbs energy of a phase φ
G_{ref}^φ	reference Gibbs energy of a phase φ
G_i^φ	partial Gibbs energy of component i in phase φ .
G_m^φ	Gibbs energy of mixing in a phase φ
G_{mi}^φ	ideal Gibbs energy of mixing in a phase φ
G_{me}^φ	excess Gibbs energy of mixing in a phase φ
G_{mc}^φ	configurational Gibbs energy of mixing in a phase φ
G_{mv}^φ	non–configurational Gibbs energy of mixing in a phase φ
$G_i^{\varphi,0}$	Gibbs energy for the pure component i in phase φ
H^φ	enthalpy of a phase φ
H_i^{SER}	enthalpy of pure component i in its stable states at 298.15 K
H_m^φ	enthalpy of mixing in a phase φ
H_{mc}^φ	configurational enthalpy of mixing in a phase φ
k_B	Boltzmann’s constant
m_i	multiplicity of cluster i
R	gas constant, $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$
S_m^φ	entropy of mixing in a phase φ
S_{me}^φ	excess entropy of mixing in a phase φ
S_{mi}^φ	ideal entropy of mixing in a phase φ
S_{mc}^φ	configurational entropy of mixing in a phase φ

S_{mv}^{φ}	non-configurational entropy of mixing in a phase φ
T	absolute temperature
u_i	the correlation function for the cluster i
u_p	the correlation function for the point cluster
x_i	mole fraction of component i

LIST OF ACRONYMS

CE	Cluster Expansion
CVM	Cluster Variation Method
CEC (ECI)	Cluster Expansion Coefficient (Effective Cluster Interaction)
CT	Computational Thermodynamics
CSA	Cluster Site Approximation
CPA	coherent potential approximation
DFT	Density Functional Theory
HEA	High Entropy alloys
1NN	First Nearest Neighbour
$(K-B)$	Kikuchi–Barker coefficients
MC	Monte Carlo
RK	Redlich–Kister
SRO	Short-Range order
SQS	Special Quasi Random Structure
SGTE	Scientific Group Thermodata Europe

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