

Analysis of Interdiffusion in Multicomponent Alloys

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Statement of the Originality

I hereby certify that the work embodied in the thesis is my own work, conducted under normal supervision. The thesis contains no material which has been accepted, or is being examined, for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made. I give consent to the final version of my thesis being made available worldwide when deposited in the University's Digital Repository, subject to the provisions of the Copyright Act 1968 and any approved embargo.

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Acknowledgement of Authorship

I hereby certify that the work embodied in this thesis contains published paper/s/scholarly work of which I am a joint author. I have included a written declaration below endorsed in writing by my supervisor, attesting to my contribution to the joint publications/scholarly work.

By signing below I confirm that Mohammad Afikuzzaman contributed (he performed calculation parts, prepared the drafts, figures and he was actively involved in the assessment of the outcomes) to the papers/ publications listed below:

Journal Article and Book Chapter

- (i) **Mohammad Afikuzzaman**, Irina V. Belova, Graeme. E. Murch and John E. Morral, “Interdiffusion analysis in ternary systems to process composition profiles and obtain constant interdiffusion coefficients using one compact diffusion couple,” *Journal of Phase Equilibria and Diffusion*, Vol 40, pp. 522-531, 2019.
- (ii) **Mohammad Afikuzzaman**, Irina V. Belova and Graeme. E. Murch, “Investigation of interdiffusion in high entropy alloys: application of random alloy model,” *Diffusion Foundations*, Vol 22, pp. 94-108, 2019.

Submitted Journal Article and Book Chapters

- (i) Irina V. Belova, **Mohammad Afikuzzaman** and Graeme. E. Murch, “A new approach for analysing interdiffusion in multicomponent alloys,” submitted to *Scripta Materialia*.
- (ii) **Mohammad Afikuzzaman**, Irina V. Belova and Graeme. E. Murch, “Novel interdiffusion analysis in multicomponent alloys. Part 1: Application to ternary alloys,” submitted to *Diffusion Foundations*.
- (iii) Irina V. Belova, **Mohammad Afikuzzaman** and Graeme. E. Murch, “Novel interdiffusion analysis in multicomponent alloys. Part 2: Application to quaternary, quinary and higher alloys,” submitted to *Diffusion Foundations*.

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Dedication

To my father, my source of inspiration, encouragement, philosophy and understanding.

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List of Symbols

Arabic Symbols	
Symbol	Description
J_i	Flux of atoms i
L_{ij}	Onsager phenomenological coefficients
X_j	Driving force
n	Number of atomic species
N	Total number of atoms
$\Delta r_{i(j)}$	Collective displacement
V	Total volume of the system
k	Boltzmann constant
T	Absolute temperature
D_i^*	Self or Tracer diffusion coefficients
$\langle r^2 \rangle$	Mean square displacement
t	Time
\tilde{D}_{ij}	Interdiffusion coefficients
D_0	Pre-exponential factor
C_i	Composition
x	Position
P	Matrix of thermodynamic factors
\tilde{d}	Matrix of the kinetic parts of the interdiffusion coefficients
f_i	Tracer correlation factor of species i
f_o	Geometrical correlation factor
f_{ii}	Diagonal collective correlation factors
$f_{ij}^{(i)}$	Off-diagonal collective correlation factor
r	Jump distance of an atom
N_i	Total number of jumps of atom i in time t
C_v	Vacancy fraction
w_i	Exchange frequency of an atom i
H_i	Vacancy escape frequency of atom i

\tilde{d}_{ii}	Diagonal interdiffusion coefficients
\tilde{d}_{ij}	Off-diagonal interdiffusion coefficients
x_M	Position of Matano plane
C_L	Composition of left end in Matano Plane
C_R	Composition of right end in Matano Plane
r_{ij}	Components of square root diffusivity
S_i	Total amount of i atoms
∇C^0	Composition gradient of component
ΔC_i	Difference of the composition vector
$[B]$	Eigenvectors
t_f	Diffusion time
M	Number of atoms per unit volume
M_0	Parameters directly related to the geometrical correlation factor

Greek Symbols	
Symbol	Description
φ	Thermodynamic factor
γ	Activity coefficients of species i
v	Velocity of the laboratory reference frame
μ_i	Chemical potential of atoms i
$[\lambda]$	Eigenvalue

Abbreviations	
Symbol	Description
HM	Hall Method
EHM	Extended Hall Method
BM	Boltzmann-Matano
SF	Sauer-Freise
fcc	Face centred cubic
bcc	Body centred cubic
hcp	Hexagonal close packed
HE	Holdsworth and Elliot
MAA	Moleko, Allnatt and Allnatt
HEA	High Entropy Alloy
MPP	Matano Plane Position
EFDM	Explicit Finite Difference Method
SIMS	Secondary Ion Mass Spectrometry
MFP	Matlab Fitting Program
SQRD	Square Root Diffusivity
MSQRD	Modified Square Root Diffusivity
MSD	Mean Square Displacement
Zn	Zinc
Co	Cobalt
Cr	Chromium
Fe	Iron
Mn	Manganese
Ni	Nickle

Abstract

Theoretical, numerical and computational modelling of the interdiffusion analysis is the major part of the diffusion and diffusion-related fields of research. In this study, general approaches for the analysis of the interdiffusion composition profiles as well as interdiffusion coefficients are investigated for solid metallic alloy systems where the number of atomic components $n \geq 3$. The main focusing of the present dissertation is to analyse the interdiffusion phenomenon for ternary, quaternary and quinary (high entropy alloys) metallic systems making use of numerically and analytically for the closed form solutions. For the ternary and quaternary metallic system composition independent interdiffusion coefficients are used mainly for the detailed study of diffusion behaviour. In quinary metallic system composition dependent (as well as composition independent) interdiffusion matrices are used for the detailed study of CoCrFeMnNi HEAs. MATLAB programming language is used as the main tool for investigating the interdiffusion phenomenon in the different metallic system. Finally, the results obtained are compared with the available experimental data.