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Alloy Phase Stability and Design

Editors: G. Malcolm Stocks, David P. Pope and Anthony F. Giamei

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MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS VOLUME 186

Alloy Phase Stability and Design

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Frontmatter
[More information](#)

Contents

PREFACE	xi
MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS	xiii
PART I: PHASE STABILITY: FIRST PRINCIPLES THEORY	
*THE ELECTRONIC STRUCTURE AND PHASE STABILITIES OF METALLIC ALLOYS	3
B.L. Györffy, A. Barbieri, D.D. Johnson, D.M. Nicholson, F.J. Pinski, W.A. Shelton, and G.M. Stocks	
FIRST-PRINCIPLES STUDY OF PHASE STABILITY IN PD-RH ALLOYS	21
D.D. Johnson, P.E.A. Turchi, Marcel Sluiter, D.M. Nicholson, F.J. Pinski, and G.M. Stocks	
GROUND STATE PROPERTIES AND MAGNETISM IN SUBSTITUTIONALLY DISORDERED Fe _{1-x} Cr _x ALLOYS	27
W.A. Shelton, Jr., F.J. Pinski, D.D. Johnson, D.M. Nicholson, and G.M. Stocks	
FIRST PRINCIPLES STUDY OF PHASE STABILITY IN THE Al-Ti SYSTEM	33
M. Asta, M. Sluiter, Prabhakar P. Singh, D. de Fontaine, T. Hong, and A.J. Freeman	
GROUND STATE PROPERTIES OF THE Al-Ti SYSTEM	41
Prabhakar P. Singh, Mark Asta, Didier de Fontaine, and Mark van Schilfgaarde	
FULL POTENTIAL LMT0 STUDY OF TiAl ALLOY	47
Pradeep K. Khowash, David L. Price, and Bernard R. Cooper	
QUANTUM-MECHANICAL ORIGINS OF COMPLEX STRUCTURES IN Al-TRANSITION METAL COMPOUNDS	53
A.E. Carlsson	
A COMPARATIVE FIRST PRINCIPLES STUDY OF PHASE STABILITY IN Ni-Ti AND Ni-Al ALLOYS AROUND EQUIATOMIC COMPOSITION	59
P.E.A. Turchi, M. Sluiter, F.J. Pinski, and D.D. Johnson	
AB INITIO CALCULATION OF THE Cu-Pd ONE-DIMENSIONAL LONG PERIOD SUPERSTRUCTURE PHASE DIAGRAM	65
G. Ceder, P. Huang, S. Menon, D. de Fontaine, D.M. Nicholson, G.M. Stocks, and B.L. Györffy	

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978-1-107-41013-8 - Materials Research Society Symposium Proceedings: Volume 186:

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Frontmatter

[More information](#)

MAGNETIC AND CHEMICAL ORDERING IN THE $NiPt$ AND THE $CoPt$ SYSTEMS J.M. Sanchez, J.L. Morán-López, and M.C. Cadeville	71
THEORETICAL INVESTIGATION OF PHASE STABILITY IN NON-MAGNETIC COPPER-NICKEL ALLOYS M. Sluiter and P.E.A. Turchi	77
A FIRST PRINCIPLES EXAMINATION OF PHASE STABILITY IN FCC-BASED $Ni-V$ SUBSTITUTIONAL ALLOYS J. Mikalopas, P.E.A. Turchi, M. Sluiter, and P.A. Sterne	83
ELECTRONIC STRUCTURE AND PHASE STABILITY PROPERTIES OF $Al-Li$ ALLOYS Antonios Gonis, Patrice E.A. Turchi, Marcel Sluiter, Frank J. Pinski, and Duane D. Johnson	89
THEORETICAL INVESTIGATION OF PHASE STABILITY IN $Ti-V$ AND $Ti-Cr$ SUBSTITUTIONAL ALLOYS M. Sluiter and P.E.A. Turchi	95
ORDER-DISORDER PHENOMENA IN COMPLEX ALLOYS: THE CASE OF Al_5 -BASED SUBSTITUTIONAL ALLOYS P.E.A. Turchi and A. Finel	101
RECENT ADVANCES IN NON SELF-CONSISTENT TOTAL ENERGY CALCULATIONS IN ALLOYS M. van Schilfgaarde, A.T. Paxton, A. Pasturel, and M. Methfessel	107
*ORDERING ENERGY OF $B2$ ALLOYS CALCULATED IN THE FROZEN POTENTIAL AND HARRIS APPROXIMATIONS W.A. Shelton, D.M. Nicholson, G.M. Stocks, F.J. Pinski, D.D. Johnson, P. Sterne, and W.M. Temmerman	113
THE ORIGIN OF POORLY CONDITIONED SUSCEPTIBILITY MATRIX WITHIN INVERSE CVM ALGORITHM IN THE CASE OF PD_3V : A COMPARISON TO THE CASE OF Ni_3V Francine Solal and Alphonse Finel	123
PART II: PHASE STABILITY: THEORY & EXPERIMENT	
*THERMODYNAMIC STABILITY OF ORDERED INTERMETALLIC COMPOUND PHASES Y. Austin Chang, Joachim P. Neumann, and Shuang-Lin Chen	131
PHASE EQUILIBRIA AND SOLIDIFICATION OF Al -RICH $Al-Li-Cu$ ALLOYS Sinn-Wen Chen and Y. Austin Chang	141
PHASE STABILITY IN BINARY $Ti-Al$ C.D. Anderson, W.H. Hofmeister, and R.J. Bayuzick	147

Invited Paper

Cambridge University Press
978-1-107-41013-8 - Materials Research Society Symposium Proceedings: Volume 186:
Alloy Phase Stability and Design
Editors: G. Malcolm Stocks, David P. Pope and Anthony F. Giamei
Frontmatter
[More information](#)

MICROSTRUCTURAL BENEFITS OF RSP IN A γ -(Ti-Ta-Al) ALLOY	155
C. McCullough, J.J. Valencia, C.G. Levi, and R. Mehrabian	
AMORPHOUS PHASE FORMATION IN NiTi DURING COLD ROLLING	161
J. Koike, D.M. Parkin, and M. Nastasi	
NANOSCALE PHASE SEPARATION INDUCED BY MECHANICAL ALLOYING IN THE IRON-ERBIUM-NITROGEN SYSTEM	169
Z. Fu, H.J. Fecht, and W.L. Johnson	
FORMATION OF CUBIC L1 ₂ PHASES FROM Al ₃ Ti AND Al ₃ Zr BY TRANSITION METAL SUBSTITUTIONS FOR Al	175
C.J. Sparks, W.D. Porter, J.H. Schneibel, W.C. Oliver, and C.G. Golec	
KINETICS OF B2 AND DO ₃ ORDERING: THEORY	181
L. Anthony and B. Fultz	
KINETICS OF ORDERING IN Fe ₃ Al: EXPERIMENT	187
Brent Fultz, Zheng-Qiang Gao, and Lawrence Anthony	
PHOTOEMISSION FROM ORDERED AND DISORDERED Cu ₃ Au	193
R.G. Jordan and B. Ginatempo	
PHOTOEMISSION MEASUREMENTS FROM NICKEL-IRON ALLOYS	199
R.G. Jordan, M.A. Hoyland, D.D. Johnson, F.J. Pinski, and J.B. Staunton	
MORPHOLOGICAL AND STRUCTURAL CHARACTERIZATION OF THE SPINODAL DECOMPOSITION OF Fe-Cr ALLOYS	203
A. Cerezo, M.G. Hetherington, J.M. Hyde, and M.K. Miller	
THE MEASUREMENT OF COMPOSITION DURING THE EARLY STAGES OF THE SPINODAL DECOMPOSITION OF Fe-Cr ALLOYS	209
M.G. Hetherington, J.M. Hyde, and M.K. Miller	
GRAIN BOUNDARY INTERMETALLIC PHASES IN ALLOY 718	215
M.G. Burke and M.K. Miller	
A STUDY OF THE PHASE DECOMPOSITION OF Fe-Ni-Al-Mo ALLOYS	219
M.K. Miller, M.G. Hetherington, J.R. Weertman, and H.A. Calderon	
ATOM PROBE ANALYSIS OF THE COMPOSITIONS OF γ' and γ'' INTERMETALLIC PHASES IN NICKEL-BASED SUPERALLOY 718	223
M.K. Miller and M.G. Burke	
THE EFFECT OF SCANDIUM ON THE PHASE STABILITY OF Al ₃ Nb AND Al ₃ Zr	229
D.M. Nicholson, J.H. Schneibel, W.A. Shelton, P. Sterne, and W.M. Temmerman	

Cambridge University Press

978-1-107-41013-8 - Materials Research Society Symposium Proceedings: Volume 186:

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Frontmatter

[More information](#)PART III: MECHANICAL PROPERTIES:
THEORY & EXPERIMENT

*ATOMISTIC MODELING OF EXTENDED DEFECTS IN METALIC ALLOYS: DISLOCATIONS AND GRAIN BOUNDARIES IN Li_2 COMPOUNDS V. Vitek, G.J. Ackland, and J. Cserti	237
INTERACTIONS BETWEEN LATTICE DISLOCATIONS AND GRAIN BOUNDARIES IN ORDERED COMPOUNDS: THEORY AND EXPERIMENT B.J. Pestman, J.Th.M. De Hosson, V. Vitek, F.D. Tichelaar, and F.W. Schapink	253
DISLOCATION CORE STRUCTURES IN NiAl R. Pasianot and D. Farkas	259
DEFORMATION AND FRACTURE BEHAVIOR OF TiAl C.L. Fu and M.H. Yoo	265
DESIGN OF HIGH ELASTIC MODULUS ALLOY USING FIRST PRINCIPLES ELECTRONIC THEORY K. Masuda-Jindo and K. Terakura	271
FIRST PRINCIPLES CALCULATIONS OF THE EQUILIBRIUM MECHANICAL PROPERTIES OF SIMPLE METALS AND ORDERED INTERMETALLIC ALLOYS Michael J. Mehl, Jean E. Osburn, Dimitri A. Papaconstantopoulos, and Barry M. Klein	277
EXTRA CONTRIBUTION OF TM SOLUTES TO THE SOLUTE-DISLOCATION/SURFACE INTERACTIONS IN NICKEL T. Shinoda, K. Masuda-Jindo, and Tomoo Suzuki	283
MECHANICAL PROPERTIES AND MICROSTRUCTURE OF CERTAIN NiAlCo(Hf) ALLOYS S.M. Russell, C.C. Law, L.S. Lin, and G.W. Levan	289
THE DISSOCIATION OF SESSILE SUPERDISLOCATIONS AT A COHERENT TWIN BOUNDARY IN ORDERED Cu_3Au DURING PLASTIC DEFORMATION F.D. Tichelaar and F.W. Schapink	295
DEFORMATION AND DISLOCATION STRUCTURE OF Ti_3Al SINGLE CRYSTALS Y. Minonishi	301
PART IV: ALLOY DESIGN: ORDERED INTERMETALLICS	
*ALLOY DESIGN OF ORDERED INTERMETALLICS E.P. George and C.T. Liu	309
DOES ϵ CONTROL INTERGRANULAR CRACKING IN Ni_3Al ? Hui Lin and David P. Pope	329

*Invited Paper

MICROSTRUCTURES OF Ni ₃ Al RAPIDLY SOLIDIFIED BY HAMMER-ANVIL TECHNIQUE Yoshinao Mishima, Shirou Sasaki, and Tomoo Suzuki	335
FRACTURE TOUGHNESS AND THE EFFECTS OF STRESS STATE ON FRACTURE OF NICKEL ALUMINIDES John J. Lewandowski, Gary M. Michal, Ivan Locci, and Joseph D. Rigney	341
DESIGNING PRECIPITATION-STRENGTHENED IRON-ALUMINIDES FOR HIGH-TEMPERATURE APPLICATIONS P.J. Maziasz, C.G. McKamey, and C.R. Hubbard	349
MICROSTRUCTURE AND COMPRESSIVE PROPERTIES OF Fe- MODIFIED L1 ₂ -TYPE Al ₃ Ti H.R. Pak, C.M. Wayman, L.H. Favrow, C.V. Cooper, and J.S.L. Pak	357
DESIGN OF L1 ₂ -TYPE Ni ₃ Si INTERMETALLICS T. Takasugi and O. Izumi	363
THE INFLUENCE OF INTERSTITIAL ALLOYING ELEMENTS ON THE PHASE STABILITY AND FRACTURE TOUGHNESS OF V ₃ Au M.A. Kassem, Y. Fahmy, and C.C. Koch	369
MECHANICAL PROPERTIES, FRACTURE BEHAVIOR, AND GRAIN- BOUNDARY CHEMISTRY OF B-DOPED NiAl E.P. George, C.T. Liu, and J.J. Liao	375
CHARACTERIZATION OF THE EFFECT OF Cr ADDITIONS TO TiAl-BASE ALLOYS Shyh-Chin Huang and Ernest L. Hall	381
PART V: ALLOY DESIGN: NICKEL BASED SUPERALLOYS, STEELS, ALUMINUM BASED ALLOYS AND GENERAL	
*ALLOY PHASE STABILITY REQUIREMENTS IN SINGLE CRYSTAL SUPERALLOYS David N. Duhl	389
INFLUENCE OF CHROMIUM AND MOLYBDENUM ON THE STRUCTURAL STABILITY OF A HIGH STRENGTH DAMAGE TOLERANT P/M NICKEL BASED ALLOY FOR TURBINE DISKS Michel Marty, Gilles Hug, and André Walder	401
SULFIDE STABILITY, VOID NUCLEATION AND THE TOUGHNESS OF ULTRA HIGH STRENGTH STEELS W.M. Garrison, Jr. and J.L. Maloney	407
ON THE STRUCTURE-PROPERTY RELATIONSHIP OF RAPIDLY SOLIDIFIED HIGH TEMPERATURE APPLICATION ALUMINUM ALLOYS A.J.S. Chowdhury and T. Sheppard	413

*Invited Paper

Cambridge University Press
978-1-107-41013-8 - Materials Research Society Symposium Proceedings: Volume 186:
Alloy Phase Stability and Design
Editors: G. Malcolm Stocks, David P. Pope and Anthony F. Giamei
Frontmatter
[More information](#)

DEVELOPMENT OF MICROSTRUCTURES WITH IMPROVED CRYOGENIC TOUGHNESS THROUGH LOCAL VARIATIONS IN STRESS STATE: ALUMINUM-LITHIUM ALLOYS	421
K.T. Venkateswara Rao and R.O. Ritchie	
DECOMPOSITION OF QUASICRYSTALLINE PHASE IN A RAPIDLY SOLIDIFIED Al-Fe-V-Si ALLOY	427
W.J. Park, S. Ahn, and N.J. Kim	
THE STABILITY OF THE $T_2(Al_6CuLi_3)$ PHASE DURING EXAMINATION IN THE TEM	433
A.S. Ramani, M.H. Tosten, C.W. Bartges, D.J. Michel, J.R. Reed, E.R. Ryba, and P.R. Howell	
PHASE STABILITY IN THE $Al_{(6-x)}Cu_xZr_2$ SYSTEM FOR $0 < x < 1$	439
P.B. Desch, R.B. Schwarz, and P. Nash	
ON THE EFFECTS OF MAGNETIC BONDING IN RARE EARTH TRANSITION METAL INTERMETALLICS	445
R. Kumar, J. Bentley, and W.B. Yelon	
AUTHOR INDEX	453
MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS	455

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Frontmatter

[More information](#)

Preface

Recent advances in the theoretical understanding of the properties of metals and alloys have opened up the possibility of a fruitful interaction with alloy design efforts. It was the intent of this symposium to bring together a wide cross-section of researchers interested in alloy design that encompassed the gamut from the quantum mechanical description of the properties of alloys to current alloy design problems. The spirit of the symposium was for researchers from the disparate fields to present their work in a manner that emphasized the connection between the underlying electronic structure and materials properties.

At the level of basic quantum theory the papers in this symposium reflect the great progress that has been made in understanding the physical properties of both ordered and disordered alloys based on Density Functional Theory (DFT). DFT provides a quantitative parameter-free (often referred to as first principles) theory of the ground state properties of these systems. This general approach has also been used in combination with classical elasticity and dislocation theory to provide the first quantitative understanding of some of the mechanical properties of intermetallic alloys. Recent advances have built on DFT theory to provide the first glimpses of a theory of the finite temperature phase stability of alloys. It is the strength of these first principles theories that the understanding of materials properties is in terms of the underlying electronic structure. At the level of atomistic simulation, based on semi-empirical potentials, again much progress has been made in understanding the properties of extended defects such as grain boundaries and dislocations. On the experimental front increasingly sophisticated tools are being brought to bear in order to understand both the underlying electronic structure and detailed atomic arrangements. This information, together with input from theory, is playing an increasing role in guiding alloy design efforts. At the more practical level a number of these sophisticated alloy design efforts have in recent years produced impressive results across a broad front. The properties of existing materials are continually being improved and new ones developed. Often this progress is based on a deeper understanding of the properties at the atomistic and electronic level. The design of new ordered intermetallic alloys that have reached or are reaching commercialization represents one of the major achievements of this investment of intellectual resources.

The papers presented at this symposium clearly demonstrate that the links between basic theory and experimentation and alloy design efforts are becoming stronger and clearly demonstrate the value of this kind of broad-based approach to materials science.

The papers in this volume cover a wide range of subjects; we have attempted to group them in some semblance of a coherent fashion. Accordingly, each section starts with one of the invited presentations. Subsequent papers in the section are grouped (roughly) to fall under the appropriate section heading.

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Frontmatter

[More information](#)

The volume contains several papers authored and co-authored by Mark Hetherington of Oxford University. Mark was tragically killed last December in an automobile accident. We would like to dedicate this proceedings to his memory. Science is the poorer for the loss of this dynamic and talented young researcher.

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Frontmatter

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Frontmatter

[More information](#)

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