Program

Fourth International Alloy Conference
(IAC-4)

The International Alloy Conferences (IACs) emphasize common elements in the experimental, theoretical, and computational study of materials properties across materials types, from metals to minerals.

June 26 - July 1, 2005

Kipriotis Village Hotel and Conference Center
Kos, Greece
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Conference Co-Chairs

A. Gonis, A. Meike, and P.E.A. Turchi
Lawrence Livermore National Laboratory

K. Rajan
Rensselaer Polytechnic Institute

ECI

Engineering Conferences International
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Engineering Conferences International (ECI) is the successor program to the United Engineering Foundation conferences program that was established in 1962 to provide an opportunity for the exploration of problems and issues of concern to engineers from many disciplines. ECI is a not-for-profit partnership between the Engineering Conferences Foundation (ECF) and Polytechnic University.

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Sunday, 26 June 2005

16:30 – 18:30  Registration
18:30 – 19:30  Reception
19:30 – 21:00  Dinner

Notes

Note that five minutes of questions and answers are allowed at the end of each presentation. Chairs are urged to keep this in mind and to remind presenters of the actual length of their talk. Participants should observe no smoking at ECI technical and social events.

During technical sessions please keep cell phones on vibrate or shut off. Take any telephone conversations out of the session room.
Monday, 27 June 2005

07:00 - 08:00  Breakfast

08:00 – 08:30  Welcome, Orientation and Information
Conference Chairs:  A. Gonis, A. Meike, P.E.A. Turchi, K. Rajan
ECI Liaison: N. Stoloff

MORNING SESSION
Chairperson: Tetsuo Mohri

08:30 – 09:00  EVALUATION OF DATA ON COARSENING IN THE FRAMEWORK
OF THE THEORY OF TRANS-INTERFACE DIFFUSION-CONTROLLED COARSENING
Alan J. Ardell, UCLA, USA

09:00 – 09:30  QUANTITATIVE PHASE-FIELD MODELING
Alphonse Finel, ONERA, France

09:30 – 10:00  GRAIN GROWTH AND TEXTURES IN NANOCRYSTALLINE FE-NI
ELECTRODEPOSITS
Y. B. Park, Sunchon National University, Korea

10:00 – 10:30  Coffee Break
Poster set up: Batt-I, Batt-II, Gadzuric, Rodriguez

Chairperson: Alan Ardell

10:30 – 11:00  THE FCC-BCC BAIN PATH IN BINARY ALLOYS UNDER HIGH
PRESSURE: VALENCE ELECTRONS AS A DRIVING FORCE
Valentina F. Degtyareva, Institute of Solid State Physics Russian
Academy of Science, Russia

11:00 – 11:30  PHYSICAL PROPERTIES OF IRON, MAX-PHASES AND SUPER-
HARD MATERIALS
Surendra K Saxena, Florida International University, USA

11:30 – 12:00  STABILITY OF HUME-ROTHERY PHASES IN CU-ZN ALLOYS AT
PRESSURES UP TO 50 GPa
Olga Degtyareva, Carnegie Institution of Washington, USA

12:00 – 17:00  Free time, ad hoc discussions
AFTERNOON SESSION

Chairperson: Dimitrios Papaconstantopoulos

17:00 – 17:30  MANY-ATOM REPULSION AND CAUCHY PRESSURE IN CUBIC SYSTEMS
                Masato Aoki, Gifu University, Japan

17:30 – 18:00  ELECRON CORRELATIONS IN RANDOM ALLOYS
                Vaclav Drchal, Institute of Physics, Czech Republic

18:00 – 18:30  THE NOTION OF EMBEDDING AND THE STUDY OF CORRELATED ELECTRONS IN MATTER
                Antonios Gonis, LLNL, USA

19:00 – 20:30  Dinner
Tuesday, 28 June 2005

MORNING SESSION

Chairperson: Anthony Paxton

07:00 - 08:30  Breakfast

08:30 – 09:00  ELECTRONIC STRUCTURE, CHEMICAL BONDING AND MECHANICAL PROPERTIES IN CRYSTALLINE AND QUASICRYSTALLINE TRANSITION-METAL ALUMINIDES
Jürgen Hafner, University of Vienna, Austria

09:00 – 09:30  REALISTIC TIGHT-BINDING METHODOLOGIES
Dimitrios A. Papaconstantopoulos, Naval Research Laboratory, USA

09:30 – 10:00  ELECTRONIC ORIGIN OF ELASTIC PROPERTIES OF TITANIUM CARBONITRIDE ALLOYS
Volodymyr I. Ivashchenko, Institute of Problems of Material Science, NAS of Ukraine

10:00 – 10:30  Coffee Break

Chairperson: J. S. Faulkner

10:30 – 11:00  MAGNETIC ALLOYS IN NANO SCALE BIOMATERIALS
Theodora Leventouri, Florida Atlantic University, USA

11:00 – 12:00  PANEL DISCUSSION ON ALLOY SCIENCE: PRESENT AND FUTURE CHALLENGES

12:00 – 17:00  Free time, ad hoc discussions

AFTERNOON SESSION

Chairperson: Antonios Gonis

17:00 – 17:30  EMBRITTLEMENT OF COPPER BY GRAIN BOUNDARY SEGREGATION OF BISMUTH
Anthony T Paxton, Queen’s University, UK

17:30 – 18:00  DISLOCATION CELL FORMATION WITHIN THE REACTION-DIFFUSION AND TDGL EQUATIONS
Tetsuo Mohri, Hokkaido University, Japan
Tuesday, 28 June 2005 (continued)

18:00 – 18:30  DISLOCATION BOUNDARY WALL GROWTH IN AL DUE TO CYCLIC HARDENING COMPARATIVE STUDY OF FATIGUE PROPERTIES OF TWO FCC METALS
M. N. Bassim, University of Manitoba, Canada

18:30 – 19:00  CRYSTAL AND DEFECT STRUCTURES OF RE SILICIDE AND ITS DERIVATIVES
Haruyuki Inui, Kyoto University, Japan

19:00 – 20:30  Dinner
Wednesday, 29 June 2005

MORNING SESSION

Chairperson: Patrice Turchi

07:00 - 08:30  Breakfast

08:30 – 09:00  CALPHAD FOR PHYSICISTS
Suzana G. Fries, SGF Scientific Consultancy, Germany

09:00 – 09:30  APPLICATION OF THE CLUSTER/SITE APPROXIMATION TO THE CALCULATION OF PHASE DIAGRAMS AND INTER-PHASE ENERGIES
Y. Austin Chang, University of Wisconsin – Madison, USA

09:30 – 10:00  FIRST-PRINCIPLES CALCULATIONS OF ALLOY PHASE DIAGRAMS BY STATISTICAL MOMENT AND CLUSTER VARIATION METHODS
Kinichi Masuda-Jindo, Tokyo Institute of Technology, Japan

10:00 – 10:30  Coffee Break

Chairperson: Marcelle Gaune-Escard

10:30 – 11:30  ACCESS TO MATERIALS CHEMISTRY AND PHASE DIAGRAM DATA. MSiT WORKPLACE
Günter Effenberg, Materials Science Internations Services GmbH, Germany

11:30 – 11:45  Group Photo

12:00 – 19:00  Free time

19:00 – 20:30  Dinner
Thursday, 30 June 2005

07:00 - 08:30  Breakfast

MORNING SESSION

Chairperson: Surendra Saxena

08:30 - 09:00  HIGH-THROUGHPUT EXPERIMENTAL APPROACHES TO STUDY ALLOY SCIENCE
J.-C. Zhao, General Electric Company, USA

09:00 - 09:30  ON THE ADVANTAGES OF USING POWDER METALLURGY IN NEW LIGHT METAL ALLOY DESIGN
Georges J. Kipouros, William F. Caley, and Paul D. Bishop, Dalhousie University, Canada

09:30 - 10:00  MECHANICAL PROPERTIES OF Ni$_2$Cr AND Ni$_2$Mo VIA FIRST-PRINCIPLES COMPUTATION
Kwai S. Chan, Southwest Research Institute, USA

10:00 - 10:30  Coffee Break

Chairperson: Jürgen Hafner

10:30 - 11:00  LATTICE STABILITY: CAN IT BE RECONCILED BETWEEN FIRST-PRINCIPLES AND CALPHAD?
Zi-Kui Liu, Pennsylvania State University, USA

11:00 - 11:30  ATOMIC ORDERING AND MAGNETISM IN L1$_0$ ORDERED FEPD ALLOYS
C. Issro, W. Pueschl, B. Sepiol, and W. Pfeiler, University of Vienna, Austria

11:30 - 12:00  ATOMIC DISPLACEMENTS IN ALLOYS
J. S. Faulkner, Florida Atlantic University, USA

12:00 - 17:00  Free time, ad hoc discussions
AFTERNOON SESSION

Chairperson: Pavel Korzhavyi

17:00 – 17:30  DFT CALCULATIONS OF PHASE STABILITIES IN THE FE-AL-C SYSTEM
Philippe Maugis, Arcelor Research, France

17:30 – 18:00  PHASE STABILITY IN GARNETS
Marcel Sluiter, Delft University of Technology, Netherlands

18:00 – 18:30  APPLICATION OF AB INITIO ELECTRONIC STRUCTURE CALCULATIONS IN PREDICTION OF STRUCTURE OF SUPERAUSTENITIC STEELS
Jan Vrestal, Masaryk University in Brno, Czech Republic

18:30 – 19:00  A COMPARATIVE STUDY OF FATIGUE PROPERTIES OF TWO FCC METALS
M. N. Bassim, University of Manitoba, Canada

19:00 – 20:30  Dinner
Friday, 1 July 2005

07:00 – 08:30  Breakfast

MORNING SESSION

Chairperson: Annemarie Meike

08:30 – 09:00  ATOMIC ORDER IN BINARY SIGMA PHASES: FE-CR, FE-V, CO-CR, AND FE-MO
Pavel A. Korzhavyi, Royal Institute of Technology (KTH), Sweden

09:00 – 09:30  ELECTRONIC STRUCTURE OF FCC AND BCC CUZN IN THE PRESENCE OF SHORT-RANGE ORDER
Derwyn Rowlands, University of Bristol, UK

10:00  Meeting Adjournment and Departure