

## ***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**

**Tel: +30-210-651-5120 Fax: +30-210-653-8674**

### **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

**Monday, 27 June 2005** (continued)

**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      **ELECTRON 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 NANOSCALE 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 **EMBRITTEMENT 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  $\text{Ni}_2\text{Cr}$  AND  $\text{Ni}_2\text{Mo}$  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  $\text{L1}_0$  ORDERED FE-PD 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

**Thursday, 30 June 2005** (continued)

**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