

Program



Peter Gumbsch
Conference Chair

**Organized by Fraunhofer-Institute for Mechanics of Materials.
Hosted by University of Freiburg.**



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Baden-Württemberg
MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST

Ministry of Science, Research and Art, Baden-Württemberg, Stuttgart, Germany

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Foreword

Computational modeling of materials behavior by multiscale materials modeling (MMM) approaches is becoming a reliable tool to underpin scientific investigations and to complement traditional theoretical and experimental approaches of component assessment. At transitional (microstructural) scales continuum approaches begin to break down and atomistic methods reach inherent limitations in time and length scale. Transitional theoretical frameworks and modeling techniques are developed to bridge the gap between the different length scales.

Industrial success in high technology fields relies on the possibility to specifically engineer materials and products with improved performance. The success factor is the ability to make these material related developments timely at relatively low-costs. This demands not only the rapid development of new or improved processing techniques but also better understanding and control of material chemistry, processing, structure, performance, durability, and their relationships. This scenario usually involves multiple length and time scales and multiple processing and performance stages, which are usually only accessible via multi-scale / multi-stage modeling or simulation.

In high-payoff, high-risk technologies such as the design of large structures in the aerospace and nuclear industries, the effects of aging and environment on failure mechanisms cannot be left to conservative approaches. Increasing efforts are now focused on advancing MMM approaches to develop new material systems components and devices. Appropriate validation experiments are crucial to verify that the models predict the correct behavior at each length scale. Thus, one of the advantages of these MMM approaches is that, at each scale, physically meaningful parameters are predicted and used in models for subsequent scales, avoiding the use of empiricism and fitting parameters.

Recent interest in nanotechnology is challenging the scientific community to design nanometer to micrometer size devices for applications in new generations of computers, electronics, photonics or drug delivery systems. These new application areas of multiscale materials modeling require novel and sophisticated science-based approaches for design and performance evaluation. Theory and modeling are playing an increasing role to reduce development costs and manufacturing times. With the sustained progress in computational power and MMM methodologies, new materials and new functionalities are increasingly more likely discovered by MMM approaches than by traditional trial and error approach. This is part of a paradigm shift in modeling, away from reproducing known properties of known materials towards simulating the behavior of hypothetical composites as a forerunner to finding real materials with these novel properties.

The MMM 2006 conference provides an international forum for the scientific advances of multiscale modeling methodologies and their applications.

I would like to thank the members of the international advisory committee, the local program committee and particularly the organizing team, the symposium organizers and the session chairs and the University of Freiburg for their engagement and support. Without their hard work and their devotion of time and resources, the Third International Conference Multiscale Materials Modeling would not have been possible.

Finally, I would like to thank our conference sponsors for their financial support: The German Research Foundation DFG, Accelrys Inc., Plansee S.E. and the Ministry of Science, Research and Art, Baden-Württemberg.

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Conference Chair

History

The first International Conference on Multiscale Materials Modeling took place at the Queen Mary University of London from June 17-20, 2002

The second International Conference on Multiscale Materials Modeling was organized by the University of California in Los Angeles from October 11-15, 2004

Conference Committees

International Advisory Committee

Prof. Bacon, David	University of Liverpool, UK
Dr. Baskes, Michael	Los Alamos National Laboratory, USA
Prof. Busso, Esteban	Imperial College, London, UK
Prof. Cale, Timothy S.	Rensselaer Polytechnic Institute, Troy, USA
Dr. Diaz de la Rubia, Tomas	Lawrence Livermore National Lab., USA
Prof. Ghoniem, Nasr	University of California, Los Angeles, USA
Prof. Guo, Xiao	Queens College, London, UK
Prof. Iwata, Shuichi	University of Tokyo, Japan
Prof. Kratochvil, Jan	Technical University, Prague, Czech Republic
Prof. Kremer, Kurt	Max Planck Institute, Mainz, Germany
Dr. Kubin, Ladislav	ONERA-LEM, Chatillon, France
Dr. LeSar, Richard	Los Alamos National Laboratory, USA
Prof. Meguid, Shaker	University of Toronto, Canada
Prof. Needleman, Alan	Brown University, Providence, USA
Prof. Odette, Robert	University of California, Santa Barbara, USA
Prof. Ortiz, Michael	California Institute of Technology, USA
Prof. Pettifor, David	Oxford University, UK
Prof. Phillips, Robert	California Institute of Technology, USA
Prof. Raabe, Dierk	Max Planck Institute, Düsseldorf, Germany
Prof. Shibusaki, Yoji	Osaka University, Japan
Dr. Soneda, Naoki	Komae Research Laboratory, Tokyo, Japan
Prof. Suresh, Subra	Massachusetts Institute of Technology, USA
Prof. Tomita, Yoshihiro	Kobe University, Japan
Prof. Van der Giessen, Erik	University of Groningen, Netherlands
Prof. Walgraef, Daniel	Free University of Brussels, Belgium
Dr. Wolf, Dieter	Argonne National Laboratory, USA
Prof. Yip, Sidney	Massachusetts Institute of Technology, USA
Dr. Zinkle, Steve	Oak Ridge National Laboratory, USA

Organizing Committee

M. J. Alava	Helsinki University of Technology, Finland
D. Dimiduk	The Ohio State University, USA
M. Dao	Massachusetts Institute of Technology, USA
M. Doi	University of Tokyo, Japan
C. Elsässer	Fraunhofer Institute for Mechanics of Materials IWM, Freiburg
E. v. d Giessen	University of Gronigen, Netherlands
N. Gov	The Weizmann Institute of Science, Israel
H. J. Herrmann	University of Stuttgart, Germany
R. James	University of Minnesota, USA
K. Kremer	Max Planck Institute for Polymer Research, Germany
J. Korvink	IMTEK, University of Freiburg, Germany
J. Li	The Ohio State University, USA
S. Müller	Max Planck Institute for Mathematics in the Sciences, Germany
A. Paxton	Queen's University, Belfast, UK
M. Payne	University of Cambridge, UK
D. Raabe	Max Planck Institute fuer Eisenforschung, Germany
N. Soneda	Central Research Institute of Electric Power Industry, Japan
M. Zaiser	University of Edinburgh, UK
S. Zapperi	University of Rome, Italy
F. Willaime	Commissariat a l'Energie Atomique (CEA), France
B. Wirth	University of California, Berkely, USA

Local Organizing Committee

P. Gumbsch	Fraunhofer Institute for Mechanics of Materials IWM, Freiburg
J. Korvink	IMTEK, University of Freiburg
C. Elsässer	Fraunhofer Institute for Mechanics of Materials IWM, Freiburg
M. Moseler	Fraunhofer Institute for Mechanics of Materials IWM, Freiburg

Logistics

Registration

Please check-in at the registration desk in the University Building II («Kollegiengebäude II») on Monday morning between 8.00 and 11.00 am. Thereafter registration is at the Information Desk in the Prometheus Hall.

Upon registration you will receive a delegate bag with all relevant documents including the conference proceedings, lunch vouchers and tickets for the conference dinner (except for students admissions).

You will also receive a badge with your name and affiliation. Your name badge will serve as admission ticket for the conference and will allow you to get lunch in the university's cafeteria. Please wear your name badge visibly throughout the conference.

Information Desk

From Tuesday thru Friday you will find the registration/information desk in the Prometheus hall on the first floor of the University Building I («Kollegiengebäude I»).

Opening and Plenary Talks

The conference opening and all plenary talks will take place in the «Audimax» in the University Building II («Kollegiengebäude II»).

Oral presentations

All symposia will be held in the University Building I («Kollegiengebäude I»). Please check the conference program for detailed information on times and exact locations of talks.

Information for speakers: Standard means of presentation will be PowerPoint. A beamer and PC laptop will be provided in each lecture hall.

Poster presentations

All posters will be displayed on Tuesday, 19 September from 5.20 to 8.00 pm and on Wednesday, 20 September from 7.00 to 9.30 pm in the Prometheus hall on the first floor and the entrance hall of the University Building I («Kollegiengebäude I»).

We are happy to announce that the Jazz Quartet «Mike Schweizer» will perform during the Wednesday poster session. There will also be a buffet for all attendees.

Mounting of posters: Tuesday, 19 September, 12.20 – 5.15 pm

Dismounting of posters: Wednesday, 20 September, 9.15 – 9.30 pm

Thursday, 21 September, 8.00 – 10.00 am

Push pins for affixing the posters to the boards will be provided by the conference organizers.

Coffee Breaks

During coffee breaks beverages and cold snacks will be provided in the Prometheus hall on the first floor of the University Building I («Kollegiengebäude I»). Coffee breaks are marked by grey bars on the conference program.

Lunch

Lunch will be offered free of charge to all conference attendees in the university's cafeteria. The cafeteria is located in Rempartstreet opposite the main entrance of University Building I (see map of conference site). You will be able to choose between three different meals including vegetarian dishes. Please use the lunch vouchers included in your delegate bags to pay for your meals. Lunch vouchers will only be valid in combination with your name badge.

Menu

Cafeteria Rempart Street

	Monday 18 September	Tuesday 19 September	Wednesday 20 September	Thursday 21 September	Friday 22 September
One-course meal	Indonesian rice dish	Green pasta (leek) in smoked salmon sauce ⁽²⁾	Goulash soup Vienna style ^(2,15) , bread roll	Nizza salad with tuna and egg, French baguette	Rice pudding with a fruit cocktail, sugar and cinnamon
Schneller Teller	<i>Indonesisches Reisgericht</i>	<i>Lauchnudeln mit Räucherlachssauce</i>	<i>Gulaschsuppe "Wiener Art" Brötchen</i>	<i>Nizzaer Salat mit Thunfisch und Ei Baguettebrötchen</i>	<i>Milchreis mit Fruchtcocktail Zucker und Zimt</i>
Meal 1	Vegetable ragout with tofu, country-potatoes, endive lettuce	Baked cheese with apple cranberry-sauce ⁽⁴⁾ , potato salad, oak-leaf lettuce	Cevapcici ⁽¹⁾ (ground meat), gipsy style, Djuvec rice, coleslaw	Cauliflower-cheese-medailon ^(4,6) , herbal dip, glazed potatoes, mixed salad	Steak, herbal dip, potatoes, lettuce
Essen 1	<i>Feines Gemüseragout mit Tofu, Country-Potatoes, Endiviensalat</i>	<i>Käsekroketten mit Apfel-Preisel-beerkompott, Kartoffelsalat, Eichblattsalat</i>	<i>Cevapcici Zigeuner Art mit Djuvecreis, Weißkrautsalat</i>	<i>Blumenkohl-Käse-Medaillon mit Kräuter-Dip, Schmelzkartoffeln, Mixsalat</i>	<i>Grünkern-Steaklet mit Kräuter-Dip und Rissoléekartoffeln, Kraussalat</i>
Meal 2	Chicken breast Caribbean style ⁽⁴⁾ , Basmati rice, carrot salad with ginger	Turkey cut into strips Kaiserstuhl style ⁽²⁾ with bread dumpling, mixed salad	Gnocchi (pasta-potato balls), Hungarian style with bell pepper sauce, lettuce, fresh fruits	Veal sausage ⁽¹⁾ , spicy sauce, french fries, lettuce	Baked salmon ⁽²⁾ garlic sauce and risotto, Iceberg salad
Essen 2	<i>Hähnchenbrust Karibische Art mit Basmatireis, Karottensalat mit Ingwer</i>	<i>Kaiserstühler Putengeschnetzeltes mit Semmelknödel, Bunter Blattsalat</i>	<i>Gnocchi "Ungarische Art" mit Paprikasauce, Kraussalat, Obst</i>	<i>Kalbsbratwurst an pikanter Gewürzsauce mit Pommes frites, Kopfsalat</i>	<i>Seelachs im Backteig mit Aiolisauce und Risotto, Eisbergsalat</i>

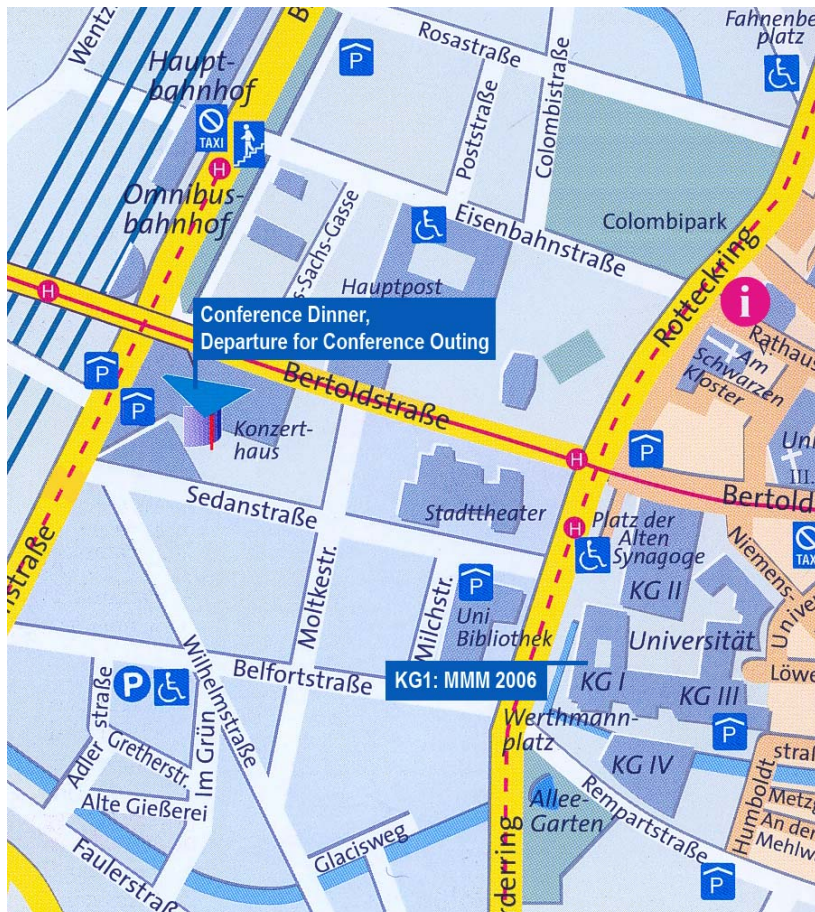
1: with porc 2: with alcohol 15: with beef 4: artificial flavor 6: artificial preserving agent

Conference Dinner

The conference dinner will take place on Thursday, 21 September at 7.30 pm in the Konzerthaus Freiburg. The dinner will be preceded by a reception at 6.30 pm. The Konzerthaus is located opposite the main train station which is five to ten minutes walk from the conference site (for detailed directions please find the map below).

Full conference admission (excl. student fees) includes a free ticket for the conference dinner which you can find in your delegate bag. Your choice of meal (vegetarian or meat) will be indicated on your ticket.

Additional tickets can be purchased for 50 € on Monday, 18 September at the conference desk. Please note that tickets are limited.



Conference Outing

The conference outing will take place on Wednesday, 20 September starting from one o'clock in the afternoon. You will have the choice between three different programs (for further details on the different programs please check our homepage at www.mmm2006.org). Please indicate your choice of program by entering your name into one of the lists displayed next to the information/registration desk in Prometheus hall.

Buses to all sites will depart at 1.10 pm from the square in front of the Konzerthaus. The Konzerthaus is located opposite the main train station which is five to ten minutes walk from the conference site (for detailed directions please find the map above). If you have already paid for the conference outing when registering for the conference you will find a ticket for the outing in your delegate bag. A limited number of additional tickets can be purchased for 20 € at the information/registration desk in Prometheus hall.

Internet Access / Hot Spots

Three PCs with internet access and Hot Spots for Wireless LAN lap tops will be available free of charge to all conference attendees. The PCs with internet connection can be found in room 1142 on the first floor of University Building I. Hot Spots will be available in room 1142 and in the Prometheus hall on the first floor of the University Building I («Kollegengebäude I»). The SSID for WLAN Access during the Conference is »MMM2006«.

Smoking

Please note that the University of Freiburg is a non-smoking area. Smoking is only permitted outside the buildings.

Conference Language

The official conference language will be English, to be used for all presentations and papers.

Venue

Street address:

Kollegengebäude I (**KGI**)
Werthmannplatz 3
79016 Freiburg
Germany

Kollegengebäude II (**KGII**)
Platz der alten Synagoge
79016 Freiburg
Germany

For a city map and further information on Freiburg please check your delegate bag.

Contact

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Conference Webpage: <http://www.mmm2006.org>

Organizing Team

Thomas Goetz
Nadine Haefner
Ulrike Zetsche
Claudia Orrelana-Rios
Franziska Schlesinger

Symposia

Symposium 1

Mathematical methods for bridging length and time scales

Organizers

R.D. James, Dept. Mechanics and Aerospace Eng., University of Minnesota, Minneapolis, USA
S. Mueller, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

Most challenging problems involve a multitude of different length and time scales and therefore cannot be attacked by brute force computation. Instead one needs to exploit the structure of the problem (including possible separation of scales) both to achieve a fundamental understanding and to design efficient numerical methods. Recently the applied mathematics community has developed a number of rigorous methods to capture the essence of fine-scale structure on the next coarser scale. At the same time a number of both heuristic and theory-inspired numerical approaches have been proposed. This Minisymposium will review both recent theoretical progress and applications to concrete problems. It will be broken down into five sessions covering:

- 1) Micromagnetics
- 2) Phase transformations
- 3) Scale bridging for the strength of materials
- 4) Bridging time scales in molecular dynamics
- 5) Soft matter

Invited Speakers

Prof. Dr. Sergio Conti	University of Duisburg, Duisburg, Germany
Prof. Dr. Ana Carpio	Universidad Complutense, Madrid, Spain
Prof. Claude Le Bris	Centre d'Enseignement et de Recherche en Mathématiques, Informatique et Calcul Scientifique (CERMICS ENPC), Marne La Vallee, France
Prof. Adriana Garroni	Universita di Roma La Sapienza, Rome, Italy
Prof. Andrea Braides	Universita di Roma, Rome, Italy
Dr. Michael Moseler	Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany
Luigi Delle Site	Max-Planck-Institute for Polymer Research, Mainz, Germany
Prof. Dominique Schryvers	University of Antwerpen, Antwerpen, Belgium
Prof. Ben Leimkuhler	University of Leicester, Leicester, UK
Dr. Simon Gill	University of Leicester, Leicester, UK
Prof. Adrian Sutton	Imperial College, London, United Kingdom
Prof. John Bassani	University of Pennsylvania, Philadelphia, USA
Prof. Richrad D. James	University of Minnesota, Minneapolis, USA
Prof. Klaus Hackl	Ruhr-Universität Bochum, Bochum, Germany
Prof. Jesus Izaguirre	Department of Computer Science and Engineering, Univ. of Notre Dame, USA
Dr. Berk Hess	Max-Planck-Institute for Polymer Research, Mainz, Germany

Symposium 2

Nanomechanics and micromechanics

Organizers

Prof. E. van der Giessen, University of Gronigen, Netherlands
Prof. M. Payne, University of Cambridge, UK

Invited Speakers

Prof. John Pethica	The University of Dublin, Trinity College, Dublin, Ireland
Prof. Adrian Sutton	Imperial College, London, United Kingdom
Prof. Nicola Marzari	Massachusetts Institute of Technology, Cambridge, USA
Prof. Markus J. Buehler	Massachusetts Institute of Technology, Cambridge, USA

Symposium 3

Statistical approaches to irreversible deformation and failure of materials

Organizers

M. J. Alava, University of Helsinki, Finland
H. J. Herrmann, ETH Zurich, Switzerland
M. Zaiser, University of Edinburgh, UK
S. Zapperi, University of Rome, Italy

During recent years, a shift in paradigm has occurred in the theory and modeling of deformation and failure of materials. Where traditional approaches focused on properties of single defects (dislocations, cracks) and on homogenization methods, a strong focus of interest is now on collective phenomena and complex spatio-temporal behavior on microscopic and mesoscopic scales. Plasticity and failure are being discussed in terms of self-similarity, scaling, and critical phenomena in non-equilibrium systems. At the same time, novel experimental approaches have been developed which give access to statistical signatures of deformation and failure on multiple length and time scales, and new systems such as non-standard crystals (vortex crystals, colloids) and amorphous solids are being investigated. The symposium aims at bringing together scientists from the statistical physics, materials science and solid mechanics communities working on irreversible materials deformation and failure. It is hoped that the exchange between researchers coming from different backgrounds, and working on different material systems, will foster 'lateral thinking' and help to develop an adequate conceptual framework for understanding complexity in deformation and failure. Equal emphasis is laid on theoretical/computational and experimental contributions, as we perceive a close collaboration between theory and experiment as a key prerequisite for any progress in this field.

List of topics to be addressed in the symposium include:

- Interacting dislocation systems: avalanches, pattern formation.
- Non-linear dynamics in plastic instabilities
- Plasticity of non conventional crystals: vortex lattices, colloidal crystals
- Irreversible deformation of non crystalline solids: glasses cohesive granular media
- Deformation-induced roughening of surfaces and interfaces
- Statistical models for fracture and plasticity at the mesoscale
- Fiber composite and fiber bundle models

Invited Speakers

Prof. Garani	Indian Institute of Science, Bangalore, India
Ananthakrishna	
Prof. Elisabeth Bouchaud	Commissariat a l'Energie Atomique (CEA), Saclay, France
Dr. Dennis Dimiduk	Air Force Research Laboratory, Ohio, USA
Prof. Phil Duxbury	Michigan State University, East Lansing, USA
Prof. Michael Falk	University of Michigan, Ann Arbor, USA
Prof. Jay Fineberg	Hebrew University, Jerusalem, Israel
Prof. J. Gil Sevillano	Centro de Estudios e Investigaciones Técnicas de Gipuzkoa (CEIT), San Sebastian, Spain
Prof. Alex Hansen	Norges Teknisk-Naturvitenskapelige Universitet (NTNU), Trondheim, Norway
Prof. Peter Hähner	JRC-EC, Ispra, Italy
Prof. Ferenc Kun	University Debrecen, Debrecen, Hungary
Prof. FrancoisLequeux	Ecole Supérieure de Physique et de Chimie Industrielles (ESPCI), Paris, France
Prof. Francois Louchet	Department of Glaciology (LGGE Grenoble), Grenoble, France
Prof. M. Carmen Miguel	University of Barcelona, Barcelona, Spain
Dr. Phani Nukala	Oak Ridge National Laboratory, Tennessee, USA
Prof. Stephane Roux	Unite Mixte du Centre National de la Recherche Scientifique (CNRS), Saint-Gobain, France
Dr. Martin Schneebeli	Eidg. Institut für Schnee- und Lawinenforschung (SLF), Davos, Switzerland
Prof. Willem Pier Vellinga	Technical University Eindhoven, Eindhoven, Netherlands
Mr. Thiebaud Richeton	Laboratoire de Glaciologie et Géophysique de l'Environnement, Saint Martin d'Hères, France
Mrs. Anne Tanguy	Université Claude Bernard, Villeurbanne, France

Symposium 4

Microstructural effects on the mechanics of materials

Organizers

D. Dimiduk, Wright Aeronautical Laboratories, Dayton, Ohio, USA
D. Raabe, Max Planck Institute, Duesseldorf, Germany

Predicting the mechanical response of materials is one of the grand challenges in multiscale materials modeling. In order to address this challenge several major issues need to be considered: accurate representations of material structure, integration of representations within simulation codes, and natural microstructure sensitivity within flow rules. This symposium focuses on emerging techniques for experimentally measuring and handling microstructural information in a way that is amenable to abstraction into multiscale materials models; representation schemes for microstructure within models; adaptive property modeling based on microstructure information; and the structure of mechanical flow rules that respond to microstructure.

Invited Speakers

Prof. Somnath Gosh	The Ohio State University, Columbus, USA
Jeff Simmons	Air Force Research Laboratory, Ohio, USA
Franz Roters	Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
Dr. Vasily Bulatov	Lawrence Livermore National Lab., University of California, Livermore, USA
Mr. Michael Groeber	The Ohio State University, Columbus, USA

Symposium 5 Biomaterials

Organizers

Prof. M. Dao, Massachusetts Institute of Technology, Cambridge, MA, USA

Prof. N. Gov, The Weizmann Institute of Science, Rehovot, Israel

Prof. J. Li, The Ohio State University, Columbus, Ohio, USA

Biological systems, such as cell, cell membrane and cytoskeleton, often consist of complex microstructures at different length scales. These subcellular microstructures are rather different from ordinary engineering materials due to the dynamic life processes. Recent developments in experimental apparatus and techniques enable evaluation of the force-displacement relationship from stretching a single DNA molecule or a whole erythrocyte with picoNewton level force resolution. While advances in computational tools in recent years have provided appealing possibilities to study the behaviour of a whole cell or its subcellular structure by incorporating appropriate molecular architecture, defect structure, and multi-scale constitutive formulations. The symposium seeks to further our understandings of the biological functions as well as disease states of a cell and its subcellular structure from a molecular-based, multiscale approach.

Invited Speakers

Prof. Subra Suresh	Massachusetts Institute of Technology, Cambridge, USA
Prof. Uzi Landman	Georgia Institute of Technology, Atlanta, USA
Prof. Dennis Discher	University of Pennsylvania, Philadelphia, USA
Prof. Sam Safran	Weizmann Institute, Rehovot, Israel
Prof. William E. Brownell	Baylor College of Medicine, Houston, USA
Prof. Agnes Ostafin	Notre Dame University, Indiana, USA
Prof. Taher Saif	University of Illinois, Urbana-Champaign, USA
Prof. Itay Rouso	Weizmann Institute, Rehovot, Israel
Prof. Helmut Schiessel	Leiden University, Leiden, Netherlands
Prof. Oded Farago	Ben-Gurion University, Beer-Sheva, Israel
Prof. Gerhard Gompper	Forschungszentrum Juelich, Juelich, Germany
Prof. Rony Granek	Ben-Gurion University, Beer-Sheva, Israel
Prof. Markus Buehler	Massachusetts Institute of Technology, Cambridge, USA
Prof. Anne Bernheim-Groswasser	Ben-Gurion University, Beer-Sheva, Israel
Dr. Markus Deserno	Max-Planck-Institut für Polymer Research, Mainz, Germany
Prof. Jay T. Groves	University of California, Berkeley, USA
Prof. N. Gov	Weizmann Institute, Rehovot, Israel

Symposium 6

Multiscale modeling of irradiation and aging of materials

Organizers

Naoki Soneda, CRIEPI, Japan

François Willaime, CEA Saclay, France

Brian D. Wirth, University of California, Berkeley, USA

Microstructural changes in materials resulting from service in environments with high-energy particle irradiation, high temperatures or cyclic thermal mechanical loads can significantly alter thermal and mechanical properties. The development of predictive performance models requires knowledge of the detailed mechanisms of defect creation and transport and the interactions amongst defect and solute/impurity species responsible for microstructure evolution, as well as the interactions between defects, solutes, impurities, and microstructural features including dislocations, grain boundaries and precipitate interfaces that control thermal and mechanical properties. Such interactions often span a very wide range of length and time scales. This symposium will provide a forum for the presentation and discussion of methods to: (1) simulate the relevant physical mechanisms at these various length and time scales, (2) treat the overlapping interfaces between these regimes, (3) create a realistic and robust multiscale approach to predicting material behavior under different exposure conditions, and (4) experimentally validate the observed phenomena.

Invited Speakers

Prof. Pascal Bellon

University of Illinois, Urbana-Champaign, USA

Prof. Alfredo Caro

Lawrence Livermore National Laboratory, CA, USA

Prof. Alfred Cerezo

University of Oxford, Oxford, UK

Jean-Paul Crocombette

Commissariat à l'Énergie Atomique (CEA), Saclay, France

Sergei Dudarev

Culham Science Centre, Oxfordshire, UK

Prof. Hideki Matsui

Tohoku University, Aoba-ku, Japan

Blas Uberuaga

Los Alamos National Laboratory, New Mexico, USA

Prof. Max Victoria

Polytechnical University of Madrid, Madrid, Spain

Dr Yury Osetskiy

Oak Ridge National Laboratory, Tennessee, USA

Symposium 7

Theoretical and experimental investigations of materials with multiple functions

Organizers

Prof. Christian Elsaesser, Fraunhofer IWM Freiburg, Germany

Prof. Anthony Paxton, Queen's University Belfast, UK

This symposium addresses the theoretical modelling and simulation as well as the experimental synthesis and characterisation of novel composite materials. They are structured on various length scales to exhibit multiple functions, and they are scientifically exciting as well as technologically promising. A few examples for such materials with multiple functions are crystalline multilayer structures with coupled ferroelectricity and ferromagnetism, surface coatings for simultaneous mechanical protection and optical tunability, flexible thin electronic displays, porous and electrostrictive light-weight metals, ferrofluidics, or nanostructured tough and ion-conducting high-temperature fuel-cell composites, etc.. Submissions of contributions are solicited, which deal with developments of innovative theoretical and experimental research techniques to create and characterise novel materials with simultaneous multiple functions on or across several length scales. The contributions may range, and preferably link, from knowledge-driven science to application-oriented development.

Invited Speakers

Dr. Ellad B. Tadmor	University of Minnesota, Minneapolis, USA
Dr. Göran Wahnström	Chalmers University of Technology, Göteborg, Sweden
PD Dr. Sibylle Gemming	University of Technology Dresden, Dresden, Germany
Dr. Simon R. Phillpot	University of Florida, Gainesville, USA
Dr. Eckhard Spohr	Forschungszentrum Juelich, Juelich, Germany
Dr. R. Ramesh	University of California, Berkeley, USA
Dr. Bernd Meyer	Ruhr-Universität, Bochum, Germany
Dr.habil. Marc Kamlah	Forschungszentrum Karlsruhe, Karlsruhe, Germany
Prof. J F Scott	University of Cambridge, United Kingdom
Dr. J M Gregg	Queen's University, Belfast, Ireland
Prof. K. Belashchenko	Nebraska Center for Materials and Nanoscience, Nebraska, USA

Symposium 8

Multiscale simulation approaches for static and dynamic properties of macromolecular materials

Organizers

Prof. K. Kremer, Max Planck Institute for Polymer Research, Mainz, Germany

Prof. M. Doi, University of Tokyo, Tokyo, Japan

Macromolecular materials inherently are governed by phenomena, which have their origin on many different time and length scales. While the dynamics of a polymer in a melt is on the one hand governed by the local bead-bead friction, providing the "prefactors" for the overall relaxation, the overall chain conformation and with this the interpenetration of the coils on a global scale play an (at least) equally important role. It is the purpose of the symposium to present and discuss recent developments in modelling approaches, which link the relevant scales and thus provide truly quantitative information of experimental and technological questions.

Invited Speakers

Prof. Florian Mueller-Plathe Technische Universitaet, Darmstadt, Germany

Prof. Doros N. Theodorou Institute of Physical Chemistry, National Centre for Scientific Research (NCRS) "Demokritos", Athens, Greece

Dr. Shiaki Hyodo Toyota Central Research Laboratory, Aichi-gun, Japan

PD. Dr. Burkhard Duenweg Max Planck Institute for Polymer Research, Mainz, Germany

Symposium 9

Materials for Micro-Electro-Mechanical Systems MEMS

Organizer

Jan G. Korvink, IMTEK, Albert-Ludwig-University Freiburg, Germany

Following the trend in microelectronics, MEMS devices are rapidly shrinking in feature size. Most of these tiny structural features are formed from IC process thin films sacrificially shaped, or by selective growth processes. Predicting material properties and behaviour requires all the tricks from the multiscaling treasury. This symposium brings together material modellers and innovators in nanostructural processing.

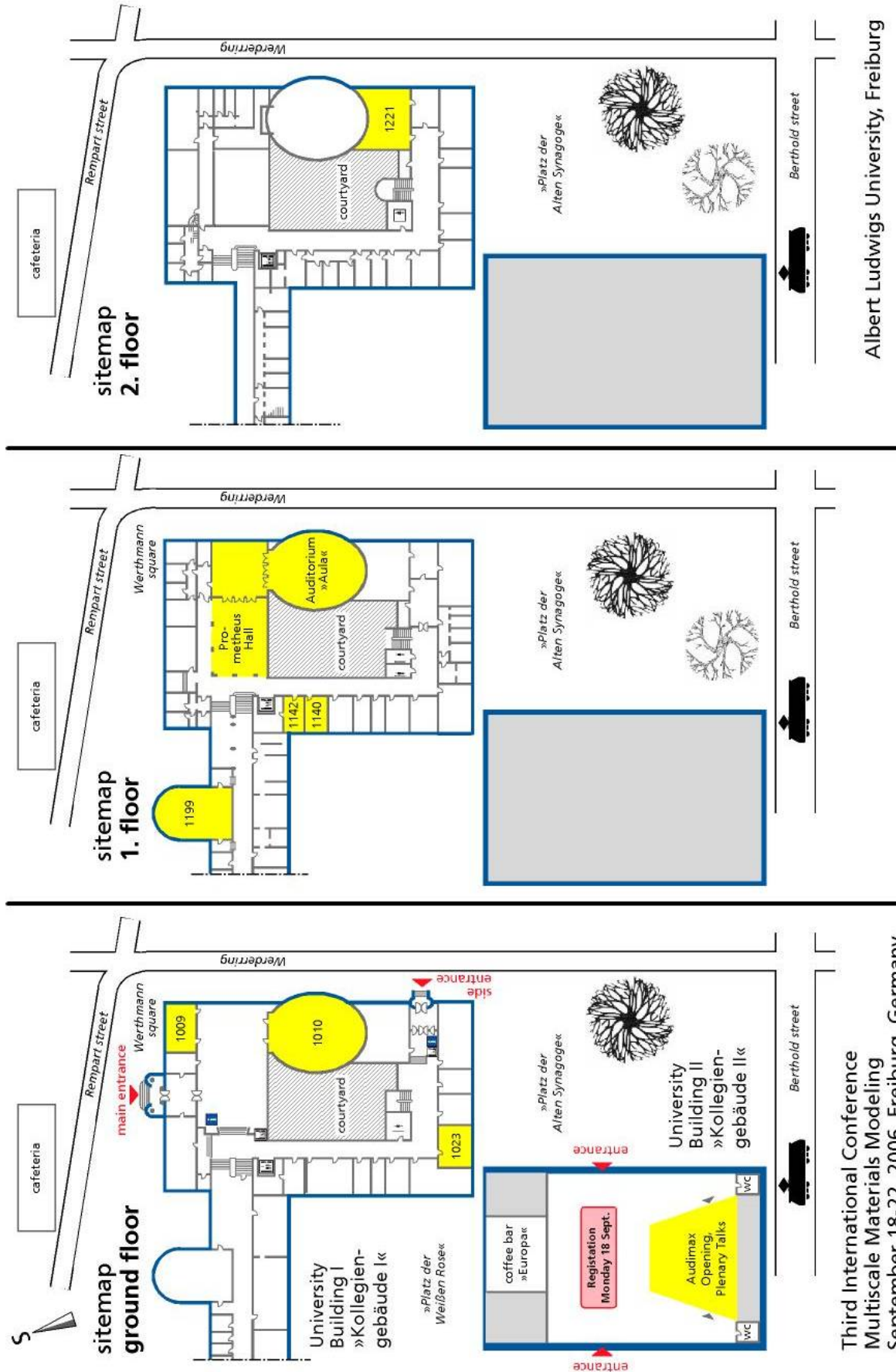
Invited Speakers

Professor Naoki Takano Ritsumeikan University, Kusatsu, Japan

Prof. Yoshitada Isono Ritsumeikan University, Kusatsu, Japan

Prof. Jürgen Wilde Department of Microsystems Engineering, University Freiburg, Freiburg, Germany

Lecture Halls



Third International Conference
Multiscale Materials Modeling
September 18-22, 2006. Freiburg, Germany

Albert Ludwigs University, Freiburg

Timetable

Monday 18 September 2006					
8.00 am	Registration from 8.00 am to 11.00 am in University Building II - Audimax				
8.20 am					
8.40 am					
9.00 am					
SESSION A PLENARY TALK AUDIMAX					
9.20 am	Opening P. Gumbsch				
9.40 am	M. Klein				
10.00 am					
10.20 am					
10.40 am	Coffeebreak in Prometheushall				
SESSION B					
	Symp. 1	Symp. 2	Symp. 4	Symp. 5	Symp. 7
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>
11.00 am	S. Conti	A. Sutton	C. Robertson	S. Suresh	R. Ramesh
11.20 am			X. Zeng		
11.40 am	J. Bassani	S. Ogata	V. Shneider	U. Landman	J.F. Scott
12.00 pm		M. Arroyo	C. Hartley		
12.20 pm	A. Garroni	M. Kalweit	Z. Wang	S. Safran	Y. Umeno
12.40 pm		G. Csanyi	J. El-Awady		G. Goldbeck-Wood
1.00 pm	Lunch in Cafeteria				
1.20 pm					
1.40 pm					
SESSION C					
	Symp. 1	Symp. 2	Symp. 4	Symp. 5	Symp. 7
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>
2.20 pm	K. Hackl	J. Pethica	F. Roters	H. Schiessel	S. Phillpot
2.40 pm					
3.00 pm	A. Carpio	M. Buehler	V. Bulatov	O. Farago	E. Spohr
3.20 pm					
3.40 pm	O. Naimark	E. Bitzek	R. Madec	N. Clauvelin	B. Ruger
4.00 pm	Coffeebreak in Prometheus hall				
SESSION C					
	Symp. 1	Symp. 2	Symp. 4	Symp. 5	
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	
4.20 pm	A. Braides	A. Hartmaier	B. Svendsen	W. Brownell	
4.40 pm		P. Pou	M.F. Wagner		
5.00 pm	P. P.-Castaneda	L. Colombo	H. Khater	N. Gov	
5.20 pm	H.D. Alber	M. Mrovec	A. Belov		
5.40 pm	A. Orlando	D. Xu	J. Llorca	A. Veksler	

Symposium 1: Mathematical methods for bridging length and time scales

Symposium 2: Nanomechanics and micromechanics

Symposium 3: Statistical approaches to irreversible deformation and failure of materials

Symposium 4: Microstructural effects on the mechanics of materials

Symposium 5: Biomaterials

Symposium 6: Multiscale modeling of irradiation and aging of materials

Symposium 7: Theoretical and experimental investigations of materials with multiple functions

Symposium 8: Multiscale simulation approaches for static and dynamic properties of macromolecular materials

Symposium 9: Materials for Micro-Electro-Mechanical Systems MEMS

Tuesday 19 September 2006						
SESSION E	Symp 1	Symp 2	Symp 4	Symp 5	Symp 6	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
9.00 am	B. Leimkuhler	N. Marzari	T. Takaki	D. Discher	P. Bellon	B. Bako
9.20 am			P.V.Sivaprasad			O. Naimark
9.40 am	V. Bulatov	R. Lebensohn	G. Singh	R. Granek	J. Lepinoux	Y.-P. Pellegrini
10.00 am	G. Lu	--	M. Hain		E. Reznikova	L. Laurson
10.20 am	Coffeebreak in Prometheushall					
SESSION F	Symp 1	Symp 2	Symp 4	Symp 5	Symp 6	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
11.00 am	S. Gill	P. Anderson	M.Starostenkov	J. Groves	B. Wirth	P. Duxbury
11.20 am		L. Colombo	D. Bentz		M. Caturla	
11.40 am	J. Izaguirre	I. Termizer	P. Jing	A. Ostafin (cancelled due to illness)	M. Caturla	M. Falk
12.00 pm		R. Kumar	J. Pan		V. Borodin	
12.20 pm	Lunch in Cafeteria					
12.40 pm						
1.00 pm						
SESSION G	Symp 1	Symp 2	Symp 4	Symp 5	Symp 6	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
1.40 pm	L. Delle Site	S. Roa	O. Kastner	T. Saif	C. C. Fu	G. Anantha-krishna
2.00 pm		N. Kioussis	J. Chaussidon		K. Wong	
2.20 pm	C. LeBris	S. B. Biner	P. Derlet	M. Buehler	M. Marinica	D. Dimiduk
2.40 pm		H.v.Swygenhofen	K. Saitoh		K. Ohsawa	
3.00 pm	E. Bitzek	D. Mordehai	H.K. Mebatsion	M. Alber	Y. Abe	F. Ciskor
3.20 am	Coffeebreak in Prometheushall					
SESSION H	Symp 1	Symp 2	Symp 4	Symp 5	Symp 6	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
3.40 pm	B. Hess	E. v.d. Giessen	V. Paidar	R. Granek	M. Andersen	F. Louchet
4.00 pm		W. Cai	V. Vitek		G. Roma	
4.20 pm	M. Moseler	J. Llorca	K. Yashiro	A.Bernheim-Groswasser	T. Bus	Th. Richeton
4.40 pm		D. Weygand	J. H. Shim		M.Starostenkov	
5.00 pm						
SESSION J	POSTER Session					
5.20 pm	Poster & Snacks (in the Prometheus hall and the entrance hall of the University Building I; 5.20 pm – 8.00 pm)					
...						
8.00 pm						

- Symposium 1: Mathematical methods for bridging length and time scales
Symposium 2: Nanomechanics and micromechanics
Symposium 3: Statistical approaches to irreversible deformation and failure of materials
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Symposium 6: Multiscale modeling of irradiation and aging of materials
Symposium 7: Theoretical and experimental investigations of materials with multiple functions
Symposium 8: Multiscale simulation approaches for static and dynamic properties of macromolecular materials
Symposium 9: Materials for Micro-Electro-Mechanical Systems MEMS

Wednesday 20 September 2006						
Session K	Symp 1	Symp 6		Symp 5	Symp 7	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>		<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
9.00 am	A. Sutton	J.P Crocombette		G. Gompper	M. Kamlah	A. Acharya
9.20 am						A. El-Azab
9.40 am	R. Drautz	B. Uberuaga		I. Rouso	R. Sviercoski	I. Groma
10.00 am	K. Scheerschmidt				--	Th. Hochrainer
10.20 am	Coffeebreak in Prometheushall					
Session L	Symp 1	Symp 2	Symp 4	Symp 5	Symp 7	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
10.40 am	A. Voigt		D. Stewart	M. Dao	E. Tadmor	M.C. Miguel
11.00 am	M. Rondanini	S. Nikolov	A. Wonisch			
11.20 am	P. Klein	P. P.-Castaneda	B. Wirth	M. Deserno	A. Sutton	M. Schneeбели
11.40 am	A. Acharya	Th. Antretter	Y. Osetskiy		S. Gemming	
12.00 pm			Y. Osetskiy	T. Auth		V. Beato
12.20 pm	Lunch in Cafeteria					
12.40 pm						
1.00 pm	Conference Outing					
1.20 pm	Departure at Konzerthaus Freiburg at 1.10 pm					
6.40 pm	Arrival at University Freiburg at 7.00 pm					
SESSION M	POSTER Session					
7.00 pm						
...	Poster & JAZZ & Buffet					
9.30 pm	(in the Prometheus hall and the entrance hall of the University Building I; 7.00 pm – 9.30 pm)					

Symposium 1: Mathematical methods for bridging length and time scales

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Symposium 9: Materials for Micro-Electro-Mechanical Systems MEMS

Thursday 21 September 2006						
SESSION N	Symp 1	Symp 6	Symp 4	Symp 8		Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>		<i>Lect.hall 1009</i>
9.00 am	R. James	M. Lavrentiev	R. Lebensohn	D.N. Theodorou		E. Bouchard
9.20 am		R. Pasianot	M. Ries			
9.40 am	J. Vilar	L. Malerba	M. Abbod	S. Hyodo		F. Lequeux
10.00 am		A. Caro	S. Berbenni			
10.20 am			C. Husson	K. Jindo		R. De
10.40 am	Coffeefreak in Prometheushall					
SESSION O	Symp 1	Symp 6	Symp 4	Symp 8		Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>		<i>Lect.hall 1009</i>
11.00 am	D. Schryvers	S. Dudarev	S. Knell	F. Mueller-Plathe		F. Kun
11.20 am			P. Maciol			
11.40 am		M. Victoria	N. Nicaise	T. Uneyama		P. Nukala
12.00 pm			M. Ronghai	G. Goldbeck-Wood		
12.20 pm		Y. Osetskiy	S. Ghosh	K. Kamio		J. G. Sevillano
12.40 pm				C. Schoen		
1.00 pm	Lunch in Cafeteria					
1.20 pm						
1.40 pm						
SESSION P	Symp 9	Symp 6	Symp 4	Symp 8	Symp 7	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1023</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
2.20 pm	Y. Isono	H. Matsui	S. Ahzi	B. Duenweg	B. Meyer	J. Fineberg
2.40 pm			F. Scheyvaerts			
3.00 pm	N. Takano	T. Nogaret	S. K. Sondhi	E. Kaxiras	J. Albina	P. Hähner
3.20 pm		E. Clouet	T. Suzudo	Y. Masubuchi	G. Wahnstrom	
3.40 pm	J. Wilde	J. Marian	S. van Boxel	C. Bretthauer		
4.00 pm		S. M. Hafez-H.	N. Zaafarani	T. Yamaue	M.G. Sob	
4.20 pm	Coffeefreak in Prometheushall					
4.40 pm						
SESSION Q	PLENARY TALK AUDIMAX					
5.00 pm	K. Kremer					
5.20 pm						
5.40 pm						
CONFERENCE DINNER in the FREIBURG KONZERTHAUS						
6.30 pm	Reception					
7.30 pm	Conference Dinner					

Symposium 1: Mathematical methods for bridging length and time scales

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Symposium 9: Materials for Micro-Electro-Mechanical Systems MEMS

	Friday 22 September 2006				
SESSION R	PLENARY TALK AUDIMAX				
9.00 am	V. Knoblauch				
9.20 am	PLENARY TALK AUDIMAX				
9.40 am					
SESSION S	Symp 9	Symp 6	Symp 4	Symp 7	Symp 3
	<i>Lect.hall 1199</i>	<i>Lect.hall 1010</i>	<i>Auditorium</i>	<i>Lect.hall 1221</i>	<i>Lect.hall 1009</i>
10.20 am	K. Annabattula	A. Cerezo	J. Simmons	J. Gregg	A. Tanguy
10.40 am	P. Berke				
11.00 am	J. Gaspar	P. Kizler	M. Groeber	F. Cleri	I. Arias
11.20 am	Coffeebreak in Prometheushall			Coffeebreak in Prometheushall	
SESSION T	Symp 9	Symp 6		Symp 7	Symp 3
	<i>Lect. hall 1199</i>	<i>Lect. hall 1010</i>		<i>Lect. hall 1221</i>	<i>Lect. hall 1009</i>
11.40 am	N. Huber	S. Yip		K. Belashchenko	W.-P. Vellinga
12.00 pm	Y. Kang	S. Nishitani			
12.20 pm		H. Kaburaki		F. Raether	S. Roux
12.40 pm				D. Tolksdorf	
1.00 pm	Lunch in Cafeteria				
	End of the Conference				

Symposium 1: Mathematical methods for bridging length and time scales

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Symposium 9: Materials for Micro-Electro-Mechanical Systems MEMS

Program

Plenary Talks

Session A

Monday, 18 September 2006

9:40 A.M.

Location: Audimax

M. Klein

Nothing Amuses More Harmlessly Than
Computation...

Proceedings Page: 3

Session Q

Thursday 21 September 2006

5:00 P.M.

Location: Audimax

K. Kremer

Multiscale Simulations of Soft Matter

Proceedings Page: 4

Session R

Friday, 22 September 2006

9:00 A.M.

Location: Audimax

V. Knoblauch

Materials Modeling: Applications, Limits and Further
Needs - An Industrial Point of View

Proceedings Page: 5

Symposium 1

Mathematical methods for bridging length and time scales

Session B

Monday, 18 September 2006

Location: lecture hall 1199

Session Chair: S. Mueller

S. Conti

Dislocation microstructures and plastic deformation of
crystals with large latent hardening

11:00 A.M. Page: 30

J. Bassani, V. Racherla

Non-Associated Flow Theory for Plastic Behavior of
Crystalline Solids

11:40 A.M. Page: 13

A. Garroni, G. Leoni

Variational models for plasticity by homogenization of
discrete dislocations

12:20 A.M. Page: 45

Session C

Monday, 18 September 2006

Location: lecture hall 1199

Session Chair: S. Conti

K. Hackl

Relaxed potentials and evolution equations

2:20 P.M. Page: 57

A. Carpio, LL. Bonilla

Discrete models of dislocations and their motion in
cubic crystals.

3:00 P.M. Page: 23

O. Naimark, V. Leont'ev, S. Uvarov

Nonlinear Dynamics of Transformation Induced
Plasticity in Shape Memory Alloys (Experimental and
Theoretical Study)

3:40 P.M. Page: 79

Session D

Monday, 18 September 2006

Location: lecture hall 1199

Session Chair: G. Dolzmann

A. Braides, L. Truskinovsky

Gamma-convergence methods for multi-scale
modeling

4:20 P.M. Page: 21

P. Ponte Castaneda

Structure-property relations for oriented and
unoriented thermoplastic elastomers

5:00 P.M. Page: 125

H. D. Alber, Z. Peicheng
Evolution of interfaces and boundaries in solids: Phase
field models
5:20 P.M. Page: 10

A. Orlando, C. Carstensen, S. Conti
Effective computation of single-slip elastoplastic
microstructures in finite strains
5:40 P.M. Page: 81

Session E

Tuesday, 19 September 2006
Location: lecture hall 1199
Session Chair: S. Mueller

B. Leimkuhler
Partial thermostating and multiple time-scale
simulation of coarse-grained MD
9:00 A.M. Page: 74

V. Bulatov, T. Opperstrup, M. H. Kalos, G. H. Gilmer,
B. Sadigh
First-passage Monte Carlo
9:40 A.M. Page: 22

G. Lu, E. B. Tadmor
From Electrons to Finite Elements: A Concurrent
Multiscale Approach
10:00 A.M. Page: 76

Session F

Tuesday, 19 September 2006
Location: lecture hall 1199
Session Chair: B. Leimkuhler

S. Gill, K. Jolley
Coupled atomistic/continuum methods for
thermoelastic problems
11:00 A.M. Page: 46

J. Izaguirre, C. R. Sweet
Backward error analysis of multiscale symplectic
integrators and propagators
11:40 A.M. Page: 65

Session G

Tuesday, 19 September 2006
Location: lecture hall 1199
Session Chair: E. Tadmor

L. Delle Site
Adaptive Resolution Molecular Dynamics Simulation:
Changing the Degrees of Freedom on the Fly
1:40 P.M. Page: 42

C. LeBris
On some microscopic stochastic models of materials
and their macroscopic limits
2:20 P.M. Page: 73

E. Bitzek, P. Koskinen, F. Gähler, M. Moseler, P.
Gumbsch
FIRE: Fast Inertial Relaxation Engine for structural
optimisations on all scales
3:00 P.M. Page: 20

Session H

Tuesday, 19 September 2006
Location: lecture hall 1199
Session Chair: A. DeSimone

B. Hess, C. Holm, N. van der Vegt
How to coarse grain ion potentials in aqueous
solutions
3:40 P.M. Page: 636

M. Moseler
Multiscale models for ion beam deposition
4:20 P.M. Page: 78

Session K

Wednesday, 20 September 2006
Location: lecture hall 1199
Session Chair: R.D. James

A. Sutton, D. R. Mason, R. E. Rudd
Atomistic Monte Carlo simulations of diffusional
phase changes
9:00 A.M. Page: 117

R. Drautz
Valence-dependent analytic bond-order potentials for
transition metals
9:40 A.M. Page: 43

K. Scheerschmidt, V. Kuhlman
Relaxation of Semiconductor Nanostructures using
Molecular Dynamics with Analytic Bond Order
Potentials
10:00 A.M. Page: 102

Session L

Wednesday, 20 September 2006
Location: lecture hall 1199
Session Chair: E. Tadmor

A. Voigt
Atomistic-continuum coupling on stepped surfaces in
epitaxial growth
10:40 A.M. Page: 119

M. Rondanini, A. Barbato, C. Cavallotti
A multiscale model of the si CVD process
11:00 A.M. Page: 98

P. Klein, P. Baumann, A. Streit
Differentiable mesoscopic fields in molecular
simulation: construction, dynamics and coupling of
length scales
11:20 A.M. Page: 69

A. Acharya
Computational Coarse-graining for the strength of materials
11:40 A.M. Page: 9

Session N

Thursday, 21 September 2006

Location: lecture hall 1199

Session Chair: A. DeSimone

R. James
Phase transformation in bacteriophage T4 tail sheath
9:00 A.M. Page: 68

J. Vilar, L. Saiz, M. Rubi
Inferring the in vivo looping properties of DNA
9:40 A.M. Page: 118

Session O

Thursday, 21 September 2006

Location: lecture hall 1199

Session Chair: S. Conti

D. Schryvers, W. Tirry, Z. Yang, B. Bartova, S. Ignacova, S. Cao, A. Srivastava
Examples of electron microscopy observations at different length scales
11:00 A.M. Page: 106

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall

and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

G. Courbebaisse, B. Chopard, J. Latt, M. Deville, O. Malaspina
The Lattice Boltzmann Method: An emergent technique for the numerical simulation of complex fluids
Poster Page: 36

C. Cupelli, B. Henrich, T. Glatzel, M. Moseler, R. Zengerle, M. Santer
Capillary Impregnation of Nano Pores
Poster Page: 37

S. Das, P. V. Sivaprasad, Utpal Borah, Baldev Raj
Mi2cell: A generic tool for linking micro features into finite element solvers
Poster Page: 41

C. Fressengeas, V. Taupin, S. Varadhan, A. J. Beaudoin
The Evolution of Excess Dislocation Density in Torsion
Poster Page: 44

T. Glatzel, C. Cupelli, U. Küster, R. Zengerle, M. Santer
Simulation of aggregating beads in microfluidics on high performance computers with a fluid particle method
Poster Page: 54

P. Lloveras
Self organized strain textures
Poster Page: 75

J. Marian
Vertical and Horizontal Communication across Scales in Materials Simulations: Strain Localization in Al
Poster Page: 77

A. Pedersen
Long Time Scale Simulations of Atomic Structure and Dynamics at Defects in Metals
Poster Page: 85

P. Popov
Multiscale modeling and simulation of fluid flows in inelastic media
Poster Page: 88

M. Qian, Z. X. Guo
Multiscale Modelling of Microstructural Evolution during Dynamic Recrystallisation coupling FEM and CA
Poster Page: 89

T. Qin, R. Drautz, D. Pettifor
Trends in the energetics of non-magnetic bcc transition metals
Poster Page: 97

I. Smolin, S. Schmauder, P. V. Makarov, R. A. Bakeyev
A micropolar framework for modeling mechanical behavior at the mesoscale with taking into account microstructure evolution
Poster Page: 112

E. Soppa, G. Fischer, J. Nellesen, V. Romanova, H. Crostack
Three-Dimensional Numerical Models Based on Tomogram
Poster Page: 116

R. Voskoboynikov
Mathematical challenges in dislocation pile-up modeling
Poster Page: 121

R. Voskoboynikov
Multi-scale modeling of dislocation pile-ups.
Poster Page: 120

N. Wellander, B. Birnir
Homogenized Maxwell's Equations; A Model for Ceramic Varistors
Poster Page: 122

L. Zhang
Studies on Meshless Thermal-Mechanical Analysis
Method
Poster Page: 123

P. Zoontjens, S. C. Hendy, T.P. Schulze
Hybrid Multiscale Modelling of the Propagation of
Grain Boundaries in Epitaxial Growth
Poster Page: 124

Symposium 2 Nanomechanics and Micromechanics

Session B

Monday, 18 September 2006

Location: lecture hall 1010

Session Chair: M. Payne

A. Sutton, T. N. Todorov
A new theory of electromigration
11:00 A.M. Page: 232

S. Ogata
Hybrid density-functional-theory/molecular-
dynamics/coarse-grained-particles simulation schemes
for reaction processes at nano-interfaces
11:40 A.M. Page: 219

M. Arroyo
Multiscale and mesoscopic modeling and simulation
of carbon nanotubes
12:00 P.M. Page: 138

M. Kalweit, D. Drikakis
Multiscale computational strategy through coupling
12:20 P.M. Page: 191

G. Csanyi
Multiscale modeling of materials systems
12:40 P.M.

Session C

Monday, 18 September 2006

Location: lecture hall 1010

Session Chair: N. Marzari

J. Pethica
Nanomechanics: New experiments in atom resolved
AFM and nanoimprint lithography
2:20 P.M. Page: 225

M. J. Buehler, H. Tang, J. Rye, A. van Duin, W.
Goddard
Multi-paradigm modeling of dynamic fracture of
silicon using ReaxFF reactive force fields
3:00 P.M. Page: 148

E. Bitzek
Atomistic Studies of Stimulated Dislocation Nucleation
at Crack Fronts
3:40 P.M. Page: 146

Session D

Monday, 18 September 2006

Location: lecture hall 1010

Session Chair: N. Marzari

A. Hartmaier
Large-scale atomistic simulations of nanoindentation:
Length-scale effects on hardness
4:20 P.M. Page: 175

P. Pou, P. Gumbsch, R. Perez
A simple model to understand the cleavage of
diamond from the bond breaking
4:40 P.M. Page: 226

L. Colombo, M. Ippolito, A. Mattoni
On the role of lattice discreteness on brittle fracture
5:00 P.M. Page: 161

M. Mrovec, Y. Cheng, C. Elsässer, P. Gumbsch
Atomistic simulations of dislocation-grain boundary
interactions in tungsten
5:20 P.M. Page: 213

D. Xu, H. Wang, R. Yang
Defect nucleation and shear instability of TiAl under
different shear condition: an atomistic simulation
5:40 P.M. Page: 248

Session E

Tuesday, 19 September 2006
Location: lecture hall 1010
Session Chair: E. van der Giessen

N. Marzari
Kinetics and thermodynamics of pressure-induced
phase transitions in semiconductor nanoparticles
9:00 A.M. Page: 208

R. Lebensohn, E. M. Bringa, A. Caro
A micromechanical study of the effect of grain size
and strain rate on the yield strength of nanostructured
materials
9:40 A.M. Page: 204

Session F

Tuesday, 19 September 2006
Location: lecture hall 1010
Session Chair: E. van der Giessen

P. Anderson, P. M. Anderson, L. Li, W. D. Nix, S. M.
Han,
Modeling Size Effects in Sub-Micron Compression
Samples
11:00 A.M. Page: 133

L. Colombo, A. Mattoni
Temperature- and strain-induced microstructure
evolution of nanocrystalline silicon
11:20 A.M. Page: 164

I. Temizer, P. Wriggers
A numerical method for homogenization in non-linear
isotropic and anisotropic elasticity
11:40 A.M. Page: 237

R. Kumar, L. Nicola, V.S. Deshpande, A. Needleman,
E. Van der Giessen
Study of the grain size dependence of plasticity in thin
films using discrete dislocation plasticity
12:00 A.M. Page: 200

Session G

Tuesday, 19 September 2006
Location: lecture hall 1010
Session Chair: M. Payne

S. Rao
3D dislocation dynamics simulations of micron-sized
fcc ni crystals
1:40 P.M. Page: 227

N. Kioussis, M. Shehadeh, G. Lu, S. Banerjee, N.
Ghoniem
Dislocation threading across Cu-Ni interface: A hybrid
atomistic-continuum approach
2:00 P.M. Page: 197

S. B. Biner, Q. Chen
Fully anisotropic 3d dislocation dynamics study of
deformation behavior in b2 intermetallic systems
2:20 P.M. Page: 142

H. Van Swygenhoven, P. M. Derlet
Life of a dislocation in a nanocrystalline fcc metal
2:40 P.M. Page: 241

D. Mordehai, G. Makov, I. Kelson
Non planar core and dynamic emission of dislocation
loops in fcc crystals
3:00 P.M. Page: 209

Session H

Tuesday, 19 September 2006
Location: lecture hall 1010
Session Chair: M. Payne

E. van der Giessen, A. Widjaja, V. S. Deshpande, A.
Needleman
On contact and size effects in discrete dislocation
modelling of wedge indentation
3:40 P.M. Page: 257

W. Cai
Plasticity and Dislocation Dynamics in Micro and
Nano-scale Cylinders
4:00 P.M. Page: 155

J. LLorca
Size effect in the flow stress of single-crystal
microbeams during bending: a dislocation dynamics
study
4:20 P.M. Page: 203

D. Weygand
Size effect in the plastic response of sub- μm sized
pillars: a three dimensional discrete dislocation
dynamics study
4:40 P.M. Page: 244

Session L

Wednesday, 20 September 2006

Location: lecture hall 1010

Session Chair: M. Payne

S. Nikolov, D. Raabe, F. Roters

A constitutive model for glassy polymers with shear transformation zones plasticity and reptation-based viscoelasticity

11:00 A.M. Page: 217

P. Ponte Castaneda

Fiber-reinforced elastomers: effective behavior, microstructure evolution and macroscopic instabilities

11:20 A.M. Page: 256

T. Antretter, T. Waitz, W. Pranger, F.D. Fischer
Prediction of the Morphology of Martensite in Nano-Structured Ni-Ti Alloys.

11:40 A.M. Page: 134

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall

and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

J. Aldazabal, J.M. Martínez-Esnaola, J. Gil Sevillano
Crack growth along symmetrical tilt grain boundaries in copper bicrystals

Poster Page: 129

C. Brandl, P.M. Derlet, H. Van Swygenhoven
Interaction of dislocations with grain boundaries in a 3D-nanocrystalline network

Poster Page: 147

M. Chabaat, S. Djouder
Contribution to the study of kinematics of the damage Zone in a brittle material

Poster Page: 156

B. Eidel, A. Stukowski
Atomistic to continuum scale transition for crystalline materials -- a comparative study of quasicontinuum approaches

Poster Page: 167

P. Gullett
An examination of local atomic deformation computed by means of a discrete gradient operator

Poster Page: 170

S. Hara, T. Kumagai, S. Izumi, S. Sakai
Atomistic simulations of dislocation-interface interactions in the fcc/hcp incoherent systems

Poster Page: 172

A. Hashibon
Atomistic Study of Structure and Failure of fcc/bcc Heterophase Boundaries

Poster Page: 254

Q. Hu, N. M. Ghoniem
Multiscale Modelling of the Early Stage of Thin Film Deposition --- from ab initio to continuum

Poster Page: 171

C. Huldt, J. Kinaret
The influence of electronic structure on a nanoelectromechanical shuttle

Poster Page: 176

T. Igarashi, S. Ogata
Development and Application of Hybrid Coarse-Grained-Particles/Molecular-Dynamics Simulation method

Poster Page: 179

S. Izumi, K. Murai, S. Hara, T. Kumagai, S. Sakai
Influence of impurity atoms on the rate of solid phase epitaxy: Molecular dynamics study

Poster Page: 183

M. Kalweit, D. Drikakis
Collision Dynamics of Nanoparticles

Poster Page: 194

I. Li, N. M. Ghoniem
Molecular Dynamics Simulations of the Mechanism of Twin Boundary Migration of Nano-twinned Copper Crystals

Poster Page: 255

S. Ogata
Energetics of bending carbon nanotube

Poster Page: 218

P. Panfilov, M. Yu. Gutkin
Intensive octahedral slip as the origin of cleavage in iridium single crystals

Poster Page: 223

L. Pastewka
An atomistic-continuum multiscale approach towards technological realization of carbon nanotube actuators

Poster Page: 224

Y. Shibutani, H. Tanaka,
Instability Analyses of Nanogrid Structures with Quasicontinuum Beam Model

Poster Page: 228

F. Siska
Finite elements computation of mechanical properties of copper thin film under tensile and cyclic loading

Poster Page: 231

A. Telezhnikov, I.L. Maksimov
Temperature Dependence of Peierls-Nabarro Barrier in Strained Crystal

Poster Page: 233

S. Yilmaz

The arrangement type of inhomogeneity considering by MTM method used for estimation of elastic moduli of particulate composites

Poster

Page: 249

T. Young, J. Kioseoglou, P. Dluwzski, P. Komninou
From 2D HRTEM images to 3D atomistic/continuum models of GaN/Al₂O₃ interfacial region

Poster

Page: 253

Symposium 3

Statistical Approaches to Irreversible Deformation and Failure of Materials

Session E

Tuesday, 19 September 2006

Location: lecture hall 1009

Session Chair: S. Zapperi

B. Bako

The Dislocation Glass

9:00 A.M.

Page: 276

O. Naimark

Structural-Scaling Transitions in Mesodeflect Ensembles as Mechanisms of Plasticity and Failure

9:20 A.M.

Page: 354

Y. Pellegrini, F. Willot, M. Idiart, P. Ponte Castaneda
Anisotropy-induced localization in 2D linear and non-linear porous materials: scaling in the dilute limit

9:40 A.M.

Page: 368

L. Laurson, M. J. Alava

1/f Noise and dislocation avalanches

10:00 A.M.

Page: 344

Session F

Tuesday, 19 September 2006

Location: lecture hall 1009

Session Chair: A. El-Azab

P. Duxbury

Rupture of polycrystalline materials

11:00 A.M.

Page: 289

M. Falk, Y. Shi

The Relationship between shear banding and the percolation of short range order in simulated amorphous solids

1:40 A.M.

Page: 296

Session G

Tuesday, 19 September 2006

Location: lecture hall 1009

Session Chair: G. Lequeux

G. Ananthakrishna

Negative strain rate sensitivity and the critical nature of type A bands in the Portevin-Le Chatelier effect

1:40 P.M.

Page: 263

D. Dimiduk, C. Woodward, M. D. Uchic, S. I. Rao, T.A. Parthasarathy

Criticality and Stochastic Flow in Microcrystal Plasticity

2:20 P.M.

Page: 282

F. Csikor

Glassy relaxation of dislocation systems

3:00 P.M.

Page: 280

Session H

Tuesday, 19 September 2006

Location: lecture hall 1009

Session Chair: F. Louchet

F. Louchet, J. Weiss, T. Richeton
The Hall-Petch law as a consequence of intermittent flow
3:40 P.M. Page: 348

T. Richeton, J. Weiss, F. Louchet, P. Dobron F. Chmelik
Critical character of plasticity from AE experiments
4:20 P.M. Page: 370

Session K

Wednesday, 20 September 2006

Location: lecture hall 1009

Session Chair: P. Haehner

A. Acharya
A Field Theory for Mesoscopic Dislocation Mechanics
9:00 A.M. Page: 271

A. El-Azab, J. Deng
Statistical characterization of dislocation ensembles
9:20 A.M. Page: 292

I. Groma, Géza Györgyi
Dynamics of coarse grained dislocation densities from an effective free energy
9:40 A.M. Page: 317

T. Hochrainer
Dislocation interactions and diffusion terms in a 3D continuum theory of dislocations
10:00 A.M. Page: 324

Session L

Wednesday, 20 September 2006

Location: lecture hall 1009

Session Chair: M. Alava

M.C. Miguel, P. Cervera, P. Moretti, S. Zapperi
Percolation of force networks and deformation properties of granular matter
10:40 A.M. Page: 352

M. Schneebeli, C. Sigrist, J. Schweizer
Failure in snow as a multiscale process
11:20 A.M. Page: 375

V. Beato
Modeling size effects in plasticity
12:00 A.M. Page: 277

Session N

Thursday, 21 September 2006

Location: lecture hall 1009

Session Chair: J. Gil Sevillano

E. Bouchaud, D. Bonamy, L. Ponson
Scaling properties of fracture surfaces
9:00 A.M. Page: 278

F. Lequeux, H. Montes
Linear and non-linear mechanics of filled elastomers, the role of the gradient of glass transition temperature
9:40 A.M. Page: 342

R. De, G. Ananthakrishna
Dynamics of the peel front and the nature of acoustic emission during peeling of an adhesive tape
10:20 A.M. Page: 281

Session O

Thursday, 21 September 2006

Location: lecture hall 1009

Session Chair: E. Bouchaud

F. Kun
Fiber models for the failure of composite materials
11:00 A.M. Page: 334

P. Nukala, S. Simunovic, S. Zapperi
Large Scale Simulation of Fracture in Disordered Media
11:40 A.M. Page: 359

J. Gil Sevillano, D. González, J. Martínez-Esnaola
Roughness of a mode in-plane crack front propagating along a heterogeneous cohesive interface in a brittle medium
12:20 P.M. Page: 310

Session P

Thursday, 21 September 2006

Location: lecture hall 1009

Session Chair: M.-C. Miguel

J. Fineberg, A. Livne
Universality and hysteretic dynamics in dynamic fracture: the rapid fracture of brittle gels
2:20 P.M. Page: 302

P. Hähner
Failure of multi-filament tows: experiments and statistical analysis
3:00 P.M. Page: 325

R. Monneau
A new kinetic formulation of dislocations dynamics
3:40 P.M.

Session S

Friday, 22 September 2006

Location: lecture hall 1009

Session Chair: F. Kun

A. Tanguy
Inhomogeneous elasto-plastic response of model
amorphous materials
10:20 A.M. Page: 383

I. Arias, J. Knap, M. Ortiz
On the Physics of Massive Crack Branching
11:00 A.M.
Page: 272

Session T

Friday, 22 September 2006

Location: lecture hall 1009

Session Chair: M. Zaiser

W. Vellinga, S. Fedorov, J. De Hosson
Fracture mechanisms on polymer-glass and polymer
metal interfaces
11:40 A.M. Page: 384

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. -8.00 P.M.

Location: Prometheus Hall
and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

S. Brochard
Atomic scale simulation study of dislocation formation
at surfaces
Poster Page: 275

I. Corominas, R. Pastor-Satorras, M.-Carmen Miguel
Percolation of force networks and deformation
properties of granular matter
Poster Page: 279

Z. Halasz, F. Kun
Fiber bundle model with stick-slip dynamics
Poster Page: 321

K. Kovacs, F. Kun
Fragments velocity distribution in impact
fragmentation
Poster Page: 326

J. Kumar, R. De, M. Ciccotti, G. Ananthakrishna
Unfolding the hidden order in acoustic emission data
in the peeling of an adhesive tape
Poster Page: 330

A. Malkin, T. Shumikhin
Statistical kinetics of quasi-brittle fracture
Poster Page: 351

N. Nikitas
Dislocation-Motivated Constitutive Equations and
Application to size effects in constrained plastic flow
Poster Page: 358

Y. Pellegrini, F. Willot
Numerical FFT computations of 2D perfectly plastic,
perfectly disordered, porous media: link between
cluster statistics and stress/strain curve
Poster Page: 369

S. Sandfeld
Continuum Theory of 3D-Dislocation Systems:
Towards a Numerical Implementation
Poster Page: 373

A. Sarkar, P. Barat and P. Mukherjee
Quantifying the Complexity of the Portevin-Le
Chatelier Effect
Poster Page: 374

J. Schwerdtfeger
Multiscale deformation patterns in single crystal
plasticity: An investigation of slip line patterns and
deformation-induced surface topography
Poster Page: 378

P. Spatig, P. Mueller, R. Bonade
Numerical investigations of the strain rate sensitivity
on the stress/strain fields
Poster Page: 379

M. Steinhauser, M. Kühn
Modelling and non-equilibrium numerical simulation
of fracture and failure in ceramics
Poster Page: 380

Symposium 4
Microstructural Effects on the Mechanics of Materials

Session B

Monday, 18 September 2006

Location: Auditorium

Session Chair: A. El-Azab

C. Robertson, J. Chaussidon, M. Fivel, K. Obrtlík, D. Rodney
Preliminary developments of 3D dislocation dynamics modelling adapted to 16MND5 ferritic steel in connection with TEM observations
11:00 A.M. Page: 510

X. Zeng, W. Blum, P. Eisenlohr
Modeling the influence of grain boundaries on deformation resistance by statistical dislocation theory
11:20 A.M. Page: 589

V. Schneider, Y. Chernyakov
The development of micro deformations theory: the account of polycrystalline material grain sizes
11:40 A.M. Page: 530

C. Hartley
On the Multipolar Character of Dislocation Distributions
12:00 P.M. Page: 451

Z. Wang, R. LeSar
Dislocation dynamics simulations of high strain rate deformation of FCC Cu
12:20 P.M. Page: 576

J. El-Awady, N.M. Ghoniem
Size Effects on the Strength of Micro-crystals
12:40 P.M. Page: 429

Session C

Monday, 18 September 2006

Location: Auditorium

Session Chair: D. Dimiduk, D. Raabe

F. Roters
Constitutive Modelling Based on Physical Mechanisms
2:20 P.M. Page: 514

V. Bulatov, V.V. Bulatov, Wei Cai, R. Cook, T. Diaz de la Rubia, J. N. Florando, M. Hiratani, G. Hommes, L. L. Hsiung, T. G. Pierce, M. Rhee, M. Tang
ParaDiS: crystal strength by direct simulation
3:00 P.M. Page: 412

R. Madec
Dislocation dynamics simulations in bcc metals
3:40 P.M. Page: 478

Session D

Monday, 18 September 2006

Location: Auditorium

Session Chair: C. Hartley

B. Svendsen, M. Henning, V. Levkovitch, H. Vehoff
Experimental investigation and multiscale modeling of orientation fields in mesocrystals
4:20 P.M. Page: 560

M. F. Wagner
Size effects on micro-twinning in NiTi shape memory alloys
4:40 P.M. Page: 575

H. Khater, D.J. Bacon, R.C. Pond, A. Serra
Multiscale Investigation of Interfacial Dislocation Mechanisms
5:00 P.M. Page: 465

A. Belov, W. Kreher
Effective domain wall-obstacle interactions for micro-mechanical modelling of ferroelectric ceramic materials
5:20 P.M. Page: 400

J. Llorca, C. González, J. Segurado
Multiscale modeling of fracture in fiber-reinforced composites
5:40 P.M. Page: 476

Session E

Tuesday, 19 September 2006

Location: Auditorium

Session Chair: F. Roters

T. Takaki, Y. Higa, Y. Tomita, A. Yamanaka
Static recrystallization simulation using phase-field model based on crystal plasticity theory
9:00 A.M. Page: 562

P. V. Sivaprasad, K.P.N. Murthy, B. Raj
A Monte Carlo study on the Nucleation and Grain growth of a polycrystalline matrix
(cancelled)
9:20 A.M. Page: 540

G. Singh, S. Amancherla, L. Jiang
Phase field coarsening model for Ni-Al-Ti ternary alloys
9:40 A.M. Page: 535

M. Hain, P. Wriggers
A micro-macro Approach for frost heave of Hardened Cement Paste and Mortar
10:00 A.M. Page: 447

Session F

Tuesday, 19 September 2006

Location: Auditorium

Session Chair: J. Simmons

M. Starostenkov, E. Dudnik
The research of thermoactivated changes of the structure of antiphase boundaries in Cu₃Au and Ni₃Al alloys
11:00 A.M. Page: 551

D. Bentz, M. Bloomfield, T. Cale, R. Gutmann, J. Lu
Stress Induced Grain Boundary Migration in Polycrystalline Via Structures
11:20 A.M. Page: 404

P. Jing, H. J. Lee, J. H. Shim, B. D. Wirth
Precipitate shape and coherency loss mechanisms in Au-Rh alloys
11:40 A.M. Page: 462

J. Pan, H. Ch'ng, R. Huang
Multiscale Modelling of Sintering
12:00 P.M. Page: 505

Session G

Tuesday, 19 September 2006

Location: Auditorium

Session Chair: A. Hartmaier

O. Kastner
Molecular dynamics of a 2D Lennard-Jones body with shape memory
1:40 P.M. Page: 463

J. Chaussidon, M. Fivel, D. Rodney
Fe-BCC plasticity at low temperature, from molecular dynamic to discrete dislocation dynamic
2:00 P.M. Page: 418

P. Derlet, C. Brandl, H. Van Swygenhoven
Constructing and characterising tailor-made grain boundary dominated structures for atomistic simulations
2:20 P.M. Page: 426

K. Saitoh
A Coarse Grain Molecular Dynamics Model of Materials Interface Using SPH and DPD Methods
2:40 P.M. Page: 518

H. K. Mebatsion, F. Mendoza, T.A. Nguyen, B.M. Nicolai, P. Verboven, B.E. Verlinden
Multiscale analysis of gas transport properties in fruits by means of microscale material models
3:00 P.M. Page: 484

Session H

Tuesday, 19 September 2006

Location: Auditorium

Session Chair: S.I. Rao

V. Paidar, A. Ostapovets
Structures and properties of planar defects in binary alloys
3:40 P.M. Page: 502

V. Vitek, R. Gröger
Effect of Non-Glide stresses on Deformation of BCC Metals at Finite Temperatures
4:00 P.M. Page: 571

K. Yashiro, J. R. Pangestu, Y. Tomita
Molecular Dynamics Study of Interfacial Dislocation Network at Gamma/Gamma-Prime Interface in Ni-Based Superalloys
4:20 P.M. Page: 582

J. Shim, Y. W. Cho, W. W. Kim, S. C. Kwon, B. Wirth
Atomistic Study of Dislocation Assisted Martensitic Transformation of Cu Precipitate in Fe
4:40 P.M. Page: 526

Session L

Wednesday, 20 September 2006

Location: Auditorium

Session Chair: V. Vitek

D. Stewart, D. Bacon, K. S. Cheong, S. Hendy, D. Knowles, Y. Osetsky
Atomic-level modelling of dislocation interactions
10:40 A.M. Page: 555

A. Wonisch, K. Korn, T. Kraft, H. Riedel
Development of Constitutive Equations for Anisotropic Sintering by Means of Micromechanical and Discrete Element Modeling
11:00 A.M. Page: 578

B. Wirth
Development of precipitate strengthening model for Cu-Co Alloys
11:20 A.M. Page: 577

Y. Osetskiy, D.J. Bacon
Atomic-scale effects in dislocation-obstacles interactions
11:40 A.M. Page: 501

Y. Osetskiy, D.J. Bacon
Strain rate and temperature effects in atomic-scale dislocation-obstacle interactions
12:00 P.M. Page: 500

Session N

Thursday, 21 September 2006

Location: Auditorium

Session Chair: S. Ahzi, S. van Boxel, Reidel

R. Lebensohn

A formulation based on Fast Fourier Transforms for the calculation of the micromechanical behavior of plastically deformed 3-D polycrystals

9:00 A.M. Page: 477

M. Ries, B. Hadler, C. Krempaszky, E. Werner
The Effect of Porosity on the Elastoplastic Behavior of High Performance-Cast Alloys

9:20 A.M. Page: 509

M. Abbod, I. Howard D. Linkens M. Mahfouf
Multi-Scale Modelling for Hot Deformation of Aluminium Alloy

9:40 A.M. Page: 393

S. Berbenni, M. Berveiller, N. Nicaise
A new micromechanical approach to account for internal lengths within plastically deforming polycrystals

10:00 A.M. Page: 408

C. Husson, S. Ahzi, F. Bilteryst, M. Oudjene
Fracture prediction in sheet metal forming process: application to the deep-drawing of OFHC copper metals

10:20 A.M. Page: 458

Session O

Thursday, 21 September 2006

Location: Auditorium

Session Chair: D. Raabe, D. Dimiduk

S. Knell, M. Sauer, K. Thoma
Mesomechanical Simulation of Elastic Wave Propagation in Al₂O₃ Ceramics

11:00 A.M. Page: 469

P. Maciol, J. Gawad, L. Madej, M. Pietrzyk
Selected Examples of Cellular Automata - Finite Element Modelling in Material Processing

11:20 A.M. Page: 479

N. Nicaise, S. Berbenni, M. Berveiller
Grain size dispersion effects on local and overall behaviours of heterogeneous materials

11:40 A.M. Page: 493

M. Ronghai, S. A. Meguid, T. Y. Ng
Nonlinear Dynamic Fe Analysis Of An Artificial Bird Striking An Aero-Engine Fan Blade

12:00 P.M. Page: 511

S. Gosh, S. Manchiraju
Multi-Time Scale Analysis of Cyclic Deformation in Polycrystalline Metals

12:20 P.M. Page: 430

Session P

Thursday, 21 September 2006

Location: Auditorium

Session Chair: S. Ghosh

S. Ahzi, H. Garmestani, S. M'Guil
Modelling Of Texture Evolution For HCP Materials Using Different Approaches (Sachs, Constrained-Hybrid, Self-Consistent, Taylor)

2:20 P.M. Page: 515

F. Schyvaerts, Y. Bréchet, P. Onck, T. Pardoen
A multiscale model for the cracking resistance of 7000 Al alloys

2:40 P.M. Page: 522

S. Sondhi, M. Henry, D. Wei
Microstructure & Property Modeling in Ni-base Superalloys

3:00 P.M. Page: 547

T. Suzudo, H. Kaburaki, Y. Fukuda, M. Itakura
A Three-Dimensional Computer Modeling on the Development of Bubbles in Polycrystalline Materials

3:20 P.M. Page: 556

S. Van Boxel, M. Seefeldt, P. Van Houtte, B. Verlinden
Slip system based model for work hardening and softening of aluminium, including strain path change effects

3:40 P.M. Page: 567

N. Zaafarani, D. Raabe, F. Roters
A study of deformation and texture evolution during nanoindentation in a Cu single crystal using phenomenological and physically-based crystal plasticity FE models

4:00 P.M. Page: 585

Session S

Friday, 22 September 2006

Location: Auditorium

Session Chair: D. Dimiduk, D. Raabe

J. Simmons, M. DeGraef, D. Dimiduk
Development of Representations of Microstructural Information Using Automated Classification and Automated Basis Function Generation Methods

10:20 A.M. Page: 534

M. Groeber, Y. Bhandari, D. Dimiduk, S. Ghosh, M. Uchic
A Framework for Creating Statistically-Equivalent Synthetic Microstructures via 3-D Microstructural Analysis

11:00 P.M. Page: 438

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall

and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

A. Al Mazouzi, M. J. Konstantinovic
Tensile properties and internal friction study of
thermal and athermal dislocation movement in Fe-Cu
alloy as a function of Cu precipitation
Poster Page: 396

M. J. Balart Murria, J. F. Knott
Microstructure-Property Relationships of
DIN22NiMoCr37 Steel in Simulated Coarse-Grained
Heat-Affected-Zone Microstructures
Poster Page: 397

M. Cerny, J. Pokluda
Influence of superimposed normal loading on the
shear strength in bcc metals
Poster Page: 414

K. Chelminski, P. Neff
Elasto-plasticity as a limit of Cosserat plasticity
Poster Page: 421

L. Colombo
Effective mechanical behavior of isotropic multi-micro-
cracked materials
Poster Page: 425

O. Gueguen, S. Ahzi, S. Belouettar, A. Makradi
New estimates of the effective elastic properties of the
semi-crystalline polyethylene
Poster Page: 497

C. Husson, S. Ahzi, J. Richeton
A yield stress model for both metals and polymers:
effects for strain rate and temperature
Poster Page: 455

N. Konchakova
Irreversible Strain and Damage in the Brittle Fracture
Materials
Poster Page: 473

J. Marian
Atomistic Study of Moving Dislocations in Disordered
Alloys
Poster Page: 483

K. Mehrabi, M. R. Rahimipour
Metallurgical Characteristics of ESR Processing in
Recovery of C300 Maraging Steel Scraps
Poster Page: 489

K. Mehrabi, M. R. Rahimipour, E. Tohidloo
The effect of Titanium content on the Microstructure
and Wear Properties of Fe-TiC Composite
Poster Page: 488

A. Misra, W. Y. Ching, J. Cheng, L. Ouyang
Relating Ab Initio Mechanical Behavior of
Intergranular Glassy Films in β -Si₃N₄ to Continuum
Scales
Poster Page: 490

J. Ocenasek, J. Alcala, O. Casals
Micromechanical Modelling of sharp indentation
experiments in single crystals and polycrystals
Poster Page: 496

T. Smorodin, M. Stecher, J. Wilde
Multiscale Physics of Failure Mechanisms in Power
Technology Metallization under Cyclic Loading
Poster Page: 544

D. Tolksdorf, H. Weckmann
Laser Post-Treatment of Plasma-Sprayed Yttrium-
Stabilized Zirconia Coatings
Poster Page: 566

Symposium 5 Biomaterials

Session B

Monday, 18 September 2006

Location: lecture hall 1023

Session Chair: N. Gov, T. Saif

S. Suresh
Computational Modeling of Cell and Molecular
Mechanics and Human Disease States
11:00 A.M. Page: 660

U. Landman
Microscopic simulations of macroscopic
consequences: fixing the continuum and hybrid
methods
11:40 A.M. Page: 642

S. Safran, A. Besser, R. De, A. Nicolas, A. Zemel
Theory of cell adhesion and elasticity
12:20 P.M. Page: 653

Session C

Monday, 18 September 2006

Location: lecture hall 1023

Session Chair: J. Groves, G. Gompper

H. Schiessel, M. Depken
From DNA to chromatin: the physics of DNA
compaction
2:20 P.M. Page: 657

Oded Farago
Meso-scale computer modeling of lipid-DNA
complexes for gene therapy
3:00 P.M. Page: 644

N. Clauvelin, S. Neukirch, B. Audoly
Analytical result for the plectonemic response of
supercoiled DNA
3:40 P.M. Page: 605

Session D

Monday, 18 September 2006

Location: lecture hall 1023

Session Chair: J. Groves, G. Gompper

W. Brownell
Electromechanical coupling in membranes
4:20 P.M. Page: 598

N. Gov, R. Shlomovitz
Membrane fluctuations driven by actin and myosin:
waves and quantized division
5:00 P.M. Page: 622

A. Veksler
Cellular shape formation driven by aggregation of
membrane proteins.
5:40 P.M. Page: 661

Session E

Tuesday, 19 September 2006

Location: lecture hall 1023

Session Chair: S. Safran, M. Buehler

D. Discher
Key roles for elasticity of matrix and cortex - from
atomistic simulation to simple thermodynamic model
9:00 A.M. Page: 614

R. Granek, A. Kahana, G. Kenan, M. Elbaum
Vibrations in Proteins: Fractons and Dynamics
Detected by Single Molecule Experiments
9:40 A.M. Page: 624

Session F

Tuesday, 19 September 2006

Location: lecture hall 1023

Session Chair: S. Safran, M. Buehler

J. Groves
Rewiring the T cell signaling network using solid-state
nanostructures
11:00 A.M. Page: 626

A. Ostafin
Scanning Probe Microscopy of Cytoskeleton Networks
(cancelled due to illness)
11:40 A.M. Page: 651

Session G

Tuesday, 19 September 2006

Location: lecture hall 1023

Session Chair: I. Rouso, M. Dao

T. Saif, S. Yang
Mechanical behavior of single living cells under stretch
and compression using micro force sensors
1:40 P.M. Page: 654

M. J. Buehler, E. Loukaides
Atomistic and continuum modeling of collagen:
Elasticity, fracture and self assembly
2:20 P.M. Page: 599

M. Alber
Multiscale Model of Morphogenesis
3:00 P.M. Page: 595

Session H

Tuesday, 19 September 2006

Location: lecture hall 1023

Session Chair: I. Rouso, M. Dao

Lecture hall 1023

R. Granek, J. Klafter
Active Transport in Disordered Microtubule Networks
3:40 P.M. Page: 623

A. Bernheim-Groswasser
Active Self-Organization Of Myosin II Motors And
Actin Filaments
4:20 P.M. Page: 597

Session K

Wednesday, 20 September 2006

Location: lecture hall 1023

Session Chair: D. Discher, A. Bernheim

G. Gompper, G. Vliegthart
Buckling and Crumpling of Virus Shells and Paper
Sheets
9:00 A.M. Page: 615

I. Rouso
The Mechanics of Retrovirus Replication Cycle
9:40 A.M. Page: 652

Session L

Wednesday, 20 September 2006

Location: lecture hall 1023

Session Chair: D. Discher, A. Bernheim

M. Dao, J. Li, S. Suresh
Molecular-Level Modeling for Erythrocyte Deformation
and Related Disease States
10:40 A.M. Page: 609

M. Deserno
Efficient simulation of coarse-grained lipid membranes
11:20 A.M. Page: 611

T. Auth, N. Gov, S. Safran
Erythrocyte membrane properties revisited
12:00 P.M. Page: 596

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall
and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

R. De
Elasticity of gels with active cells
Poster Page: 610

Symposium 6
Multiscale Modeling of Irradiation and Ageing of
Materials

Session E

Tuesday, 19 September 2006

Location: lecture hall 1221

Session Chair: n.N.

P. Bellon, A. Badillo, Y. Liu, P. Krasnochtchekov, R. S.
Averback
Generalized phase field modeling for microstructural
evolutions in irradiated materials
9:00 A.M. Page: 679

J. Lepinoux
Validation of an improved Cluster Dynamics method
based on Monte Carlo inputs
9:40 A.M. Page: 740

E. Reznikova, V. Nazmov, J. Mohr, A. Last
Physical-chemical investigation and modeling of
netlike polymerization of negative SU-8 resist during
X-ray lithography processes
10:00 A.M. Page: 788

Session F

Tuesday, 19 September 2006

Location: lecture hall 1221

Session Chair: n.N.

Lecture hall 1221

B. Wirth, P. R. Monasterio, G. R. Odette
Kinetic Monte Carlo modeling of cascade aging and
damage accumulation in Fe-Cu alloys
11:00 A.M. Page: 812

M. Caturla, C.J. Ortiz
Spatial correlation effects in irradiated materials: rate
theory vs. kinetic Monte Carlo simulations
11:20 A.M. Page: 695

M. Caturla, C.C. Fu, C. J. Ortiz, F. Willaime
Influence of carbon impurities on He migration and
clustering in -Fe
11:40 A.M. Page: 699

V. Borodin, P.V. Vladimirov, A. Möslang
Monte Carlo simulation of helium thermal desorption
from bcc iron
12:00 P.M. Page: 688

Session G

Tuesday, 19 September 2006

Location: lecture hall 1221

Session Chair: n.N.

C. C. Fu, E. Meslin, A. Barbu, F. Gao, F. Willaime
Atomic transport via interstitials in dilute Fe-P alloys
1:40 P.M. Page: 725

K. Wong, J.H. Shim, B.D. Wirth
Modeling point defect interactions in pure Fe and Fe-Cr alloys
2:00 P.M. Page: 815

M. C. Marinica, F. Willaime
Combining ab initio and empirical potential calculations to study interstitial clusters in alpha-iron
2:20 P.M. Page: 759

K. Ohsawa, E. Kuramoto
Equilibrium structure and thermal activation of dislocation loops in BCC metals
2:40 P.M. Page: 779

Y. Abe, H. Matsui
Effect of undersized Fe atoms on dynamic behavior of interstitial configuration near an edge dislocation in V using molecular dynamics simulation
3:00 P.M. Page: 665

Session H

Tuesday, 19 September 2006

Location: lecture hall: 1221

Session Chair: n.N.

M. Andersen, N. M. Ghoniem
Surface Roughening Mechanisms for Tungsten Exposed to Laser, Ion, and X-ray Pulses
3:40 P.M. Page: 670

G. Roma
A First Principles Study of Palladium in Silicon Carbide
4:00 P.M. Page: 787

T. Bus, Brian D. Wirth, Yutai Katoh, Lance L. Snead
The impact of point defects, small clusters and dislocations on the thermal conductivity and dimensional stability of 3C-SiC
4:20 P.M. Page: 692

M. Starostenkov, G. M. Poletaev, N. Cholodova
Point defects and their influence on thermoactivated disordering process of Ni3Al intermetallide
4:40 P.M. Page: 792

Session K

Wednesday, 20 September 2006

Location: lecture hall 1010

Session Chair: n.N.

J. P. Crocombette, A. Chartier, W. J. Weber
Atomistic simulation of amorphization thermo-kinetics in lanthanum pyrozoirconate
9:00 A.M. Page: 712

B. Uberuaga
Structure and Mobility of Radiation-induced Defects in MgO
9:40 A.M. Page: 797

Session N

Thursday, 21 September 2006

Location: lecture hall: 1010

Session Chair: n.N.

M. Lavrentiev, D. Nguyen-Manh, R. Drautz, P. Klaver, S.L. Dudarev
Cluster expansion-based Monte Carlo simulations of Fe-Cr solid solution
9:00 A.M. Page: 744

R. Pasianot, G. Bonny, L. Malerba
Interatomic potentials consistent with thermodynamics: The cases of FeCu and FeCr
9:20 A.M. Page: 783

L. Malerba, D. A. Terentyev, P. Olsson
Influence of Cr content on the microstructural evolution of electron irradiated Fe-Cr binary alloys: a multiscale modelling study
9:40 A.M. Page: 748

A. Caro, E. M. Lopasso, M. Caro, D. A. Crowson, S. G. Srivilliputhur
Modeling radiation damage in FeCr alloys
10:00 A.M. Page: 693

Session O

Thursday, 21 September 2006

Location: lecture hall: 1010

Session Chair: n.N.

S. Dudarev, P.M. Derlet
Interatomic potentials for materials with interacting electrons
11:00 A.M. Page: 713

M. Victoria
Modeling the effects of irradiation and the need for experimental validation
11:40 A.M. Page: 809

Y. Osetskiy, R.E. Stoller, S. Zinkle
Atomic-scale mechanisms of cleared channels formation in neutron-irradiated fcc metals.
12:20 A.M. Page: 782

Session P

Thursday, 21 September 2006

Location: lecture hall: 1010

Session Chair: n.N.

H. Matsui
2:20 P.M.

T. Nogaret, C. Robertson, D. Rodney
MD simulations and TEM observations in ion-irradiated austenitic stainless steels.
3:00 P.M. Page: 774

E. Clouet, D. Mordehai
The vacancy-edge dislocation interaction in fcc metals
3:20 P.M. Page: 708

J. Marian
A Dislocation Dynamics Approach for fcc Metals:
Implementation of Partial Dislocations
3:40 P.M. Page: 758

S. M. Hafez Haghghat, R. Schaeublin
Molecular dynamics modeling of cavity strengthening
in irradiated iron
4:00 P.M. Page: 729

Session S

Friday, 22 September 2006

Location: lecture hall 1010

Session Chair: n.N.

A. Cerezo, S. Hirose, A. Morley, G. Sha, G. D.W.
Smith
3-D atomic-scale experimental and modelling studies
of copper precipitation in low alloy steels
10:20 A.M. Page: 703

P. Kizler, C. Kohler, P. Binkele, D. Willer, T. Al-Kassab
Ageing of steels by nucleation and growth of Cu
precipitates - understood by a synopsis of various
experimental methods, molecular dynamics and
Monte-Carlo simulations of energy minimization
11:00 A.M. Page: 736

Session T

Friday, 22 September 2006

Location: lecture hall 1010

Session Chair: n.N.

S. Yip, T. Zhu, J. Li
Atomistic Measures of Strength, Deformation and
Reactivity: Toward Multiscale Modeling of Chemo-
Mechanical Phenomena
11:40 A.M. Page: 816

S. Nishitani, A. Seko, K. Yuge, I. Tanaka
Vacancy effect on the precipitate nucleation in Fe-Cu
alloy
12:00 P.M. Page: 771

H. Kaburaki, M. Yamaguchi, Y. Nishiyama, M. Shiga,
H. Matsuzawa
Impurity-induced decohesion in iron grain boundary -
A first-principles study -
12:20 P.M. Page: 733

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall

and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

A. Al Mazouzi, M. Jardin, M. Lambrecht and L.
Malerba
On the correlation between microstructure and
hardening evolution under irradiation of low Cu RPV
steel in comparison with model alloys
Poster Page: 669

C. Arevalo, M. J. Caturla, J. M. Perlado
Microstructure evolution for fission reactor cladding
formed by zirconium alloys: application to Monte
Carlo simulations
Poster Page: 671

S. Barannikova, L. B. Zuev, S. A. Barannikova, V. I.
Danilov
On the direct relationship between macroscopic
phenomena of plastic flow localization and solids
microcharacteristics
Poster Page: 675

P. Bellon, A. Badillo, Y. Liu, P. Krasnochtchekov, R. S.
Averback
Phase field modeling of the evolution of composition
in a binary alloy under irradiation
Poster Page: 687

Y. Cheng, M. Mrovec, P. Gumbsch
Crack nucleation from dislocation-grain boundary
interaction in tungsten
Poster Page: 704

Y. Cheng, M. Mrovec, P. Gumbsch
Dislocation interaction with the local stress field of
a Σ 9 tilt grain boundary in tungsten
Poster Page: 705

F. Djurabekova, R. Domingos, G. Cerchiara, N. Castin,
L. Malerba
Artificial intelligence applied to atomistic kinetic
Poster Page: 721

C. C. Fu, A. Barbu, J.L. Bocquet, L. Joly, F. Willaime
Defect kinetics in electron irradiated steels: a
multiscale modelling
Poster Page: 724

M. Gilbert, S. L. Dudarev, P. M. Derlet, D. G. Pettifor
Stability of open and collapsed vacancy type clusters
in bcc iron
Poster Page: 726

L. Malerba, C. Becquart, C. Domain
Object kinetic Monte Carlo study of sink strengths
Poster Page: 755

- L. Malerba, G. U. Bonny, D. A. Terentyev, P. Olsson, C. Domain
Ordering and clustering in Fe-Cr binary alloys: an atomistic simulation study
Poster Page: 752
- F. Mota, M. J. Caturla, J. Molla, J. M. Perlado, A. Ibarra
Defects produced in irradiated fused silica: influence of hydrogen concentration
Poster Page: 760
- O. Naimark, S. Permyakov, V. Leont'ev, Y. Bajandin, V. Oborin
Collective modes of mesodefects and "slow dynamics" of damage-failure transition in materials
Poster Page: 764
- K. Nakashima, A. Nomoto, N. Soneda, K. Ogata, K. Kamimura
Point defect diffusion in Zirconium under tensile strain
Poster Page: 766
- D. Nguyen-Manh, M. Lavrentiev, S. Dudarev
Magnetic properties of point defects and nano-clustering in Fe-Cr alloys: a systematic ab initio study
Poster Page: 767
- A. Nomato, N. Sonda, A. Takahashi
SIA-loop transformation and growth by cascade overlapping in bcc Fe
Poster Page: 778
- R. Novokshanov
Dislocation dynamics model of the stability under loading of $\langle 111 \rangle$ prismatic loops in iron
- L. Pillon, C. Denoual, R. Madec, Y.P. Pellegrini
Influence of inertia on dislocation dipoles strength
Poster Page: 786
- M. Samaras, P. M. Derlet, H. Van Swygenhoven, M. Victoria
Atomistic simulations of irradiated magnetic nanocrystalline iron
Poster Page: 790
- D. Srinivas S
Modeling of Irradiation of Titanium Powder With Nd:YAG Laser
Poster Page: 789
- M. Starostenkov
The stability of vacancy clusters in fcc crystals
Poster Page: 791
- E. Tarleton
2-dimensional dislocation dynamics modelling of brittle-ductile transitions in bcc metals
- D. Terentyev, L. Malerba, P. Olsson
Influence of Cr content on the microstructural evolution of electron irradiated Fe-Cr binary alloys: a multiscale modelling study
Poster Page: 796
- L. Ventelon, F. Willaime
Ab initio study of the core structure and mobility of screw dislocations in \pm -Fe
Poster Page: 805
- R. Voskoboynikov
Interdependent nucleation of self-interstitial and vacancy clusters in displacement cascades in Cu.
Poster Page: 810
- F. Willaime, G. Verite, C.C. Fu
Stability and mobility of self-interstitials in hcp-Zr from first principles
Poster Page: 811
- B. Wirth, H. Jee Lee, L. Saintoyant
MD simulations of dislocation interactions with stacking fault tetrahedron and Frank loops in Cu
Poster Page: 813
- B. Wirth, H. Jee Lee, B. Sadigh, J. Hyeok Shim, K. Wong
Modeling radiation damage evolution in Fe-Cr alloys
Poster Page: 814

Symposium 7
Theoretical and Experimental Investigations of
Materials with Multiple Functions

Session B

Monday, 18 September 2006

Location: lecture hall 1221

Session Chair: C. Elsaesser

M. Alexe, R. Ramesh
Correlated oxide heterostructures and nanostructures
11:00 A.M. Page: 868

J. F. Scott, N. D. Mathur, W. Eerenstein, G. Catalan,
M. Daraktchev
Studies of some Multiferroic Materials
11:40 A.M. Page: 871

Y. Umeno, C. Elsaesser, B. Meyer, P. Gumbsch, T.
Shimada, T. Kitamura
Ab initio DFT study on ferroelectricity in perovskite
surface and multilayer
12:20 P.M. Page: 901

G. Goldbeck-Wood
Advancing Multiscale Materials Modeling in the
Nanotechnology Consortium
12:40 P.M. Page: 843

Session C

Monday, 18 September 2006

Location: lecture hall 1221

Session Chair: A.T. Paxton

S. Phillpot, I. Jang, P. Barry, W. Sawyer, S. Sinnott
Tribology in polytetrafluoroethylene from molecular
dynamics simulation
2:20 P.M. Page: 862

E. Spohr
Proton Generation and Transport in the Fuel Cell
Environment. Atomistic Computer Simulations
3:00 P.M. Page: 878

B. Ruger, D. Fouquet, A. Weber, E. Ivers-Tiffee, V.
Heuveline
Micro-Modeling of solid-oxide-fuel-cell electrodes
3:40 P.M. Page: 870

Session K

Wednesday, 20 September 2006

Location: lecture hall 1221

Session Chair: C. Elsaesser

M. Kamlah, D. Zhou, B. Laskewitz
Ferroelectrics: Experiments, Micromechanics, and
Constitutive Modeling
9:00 A.M. Page: 851

R. Sviercoski, B. J. Travis
Analytical Effective Coefficient for Flow Equations in Porous
Media by homogenization theory
9.40 A.M. Page: 885

Session L

Wednesday, 20 September 2006

Location: lecture hall 1221

Session Chair: A.T. Paxton

E. Tadmor, R. Elliott, M. Dobson
A Quasicontinuum for Complex Crystals
10:40 A.M. Page: 889

A. Sutton, G. Pruessner, S. von Althaus, K.K. Kaski,
P.D. Haynes
Grain boundaries in silicon - a new look at an old
problem
11:20 A.M. Page: 884

S. Gemming
Modelling Ferroic Functional Elements
11:40 A.M. Page: 835

Session P

Thursday, 21 September 2006

Location: lecture hall 1221

Session Chair: C. Elsaesser

B. Meyer
Modeling Surfaces, Interfaces and Compositional
Order in Ferroelectric Materials
2.20 P.M. Page: 861

J. Albina, M. Mrovec, B. Meyer, C. Elsasser
A theoretical study of the semi-coherent
SrTiO₃/SrZrO₃ interface by first-principles calculations
3:00 P.M. Page: 819

G. Wahnstrom, M. Christensen, S. Johansson
Metal-ceramic interfaces from first-principles
3:20 P.M. Page: 905

M. Sob, J. Houserova, J. Vrestal, A. Kroupa
Application of ab initio electronic structure
calculations in construction of phase diagrams of
complex systems
4:00 P.M. Page: 877

Session S

Friday, 22 September 2006

Location: lecture hall 1221

Session Chair: A.T. Paxton

J.M. Gregg
Measurement and Rationalisation of Domain
Periodicities in Nanoscale Ferroics and Multiferroics
10:20 A.M. Page: 847

F. Cleri, S. Letardi
Functionalized molecular monolayers contacted to
silicon surfaces
11:00 A.M. Page: 826

Session T

Friday, 22 September 2006

Location: lecture hall 1221

Session Chair: C. Elsaesser

K. Belashchenko

First-principles modeling of spin-dependent tunneling
in magnetic tunnel junctions

11:40 A.M.

F. Raether

Simulation of thermoelastic and electrical properties
of sintered ceramics

12:20 P.M.

Page: 867

D. Tolksdorf, E. Westkämper

Developments in precision product manufacturing for
laser-sintering

12:40 P.M.

Page: 897

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall

and

Poster Session M

Wednesday 20 Sept. 2006, 7:00 P.M. – 9.30 P.M.

Location: Prometheus Hall

B. Ao, X. Wang, J. Yang, W. Hu, J. Xia

Atomic-scale simulation of helium bubbles in
aluminium

Poster

Page: 823

D. Cole, M. C. Payne, L. Colombi Ciacchi

Development of a classical force field for the
simulation of solvated proteins on oxidised and
hydroxylated silicon surfaces

Poster

Page: 830

I. Cole

Use of Multi-scale modelling to predict the
degradation of metals in real environments

Poster

Page: 831

R. S. Elliott

A Multiscale Stability Criterion for Multilattice Crystals

Poster

Page: 833

L. Elsoufi, W. Charon, M. Zoaeter, K. Khalil, R. Lachat

Methodology of thermo-mechanical tests, for the
characterization of the stiffness increment of a
multilayer piezoelectric actuator under the effect of
temperature increment

Poster

Page: 832

J. Fan

Multi-scale Analysis of the Portevin-Le-Chatelier-
Effects in annealed and solution-treated Al-4%Cu-
alloys

(cancelled)

Poster

Page: 834

R. Iglesias, S. L. Palacios

Ab initio studies of the magnetic phase stability of
iron

Poster

Page: 848

R. Kozubski, A. Biborski

Triple defect and constitutional vacancies in b2
binaries direct bragg - Williams thermodynamics

Poster

Page: 854

D. Legut, M. Sob

The study of magnetism and the ideal tensile strength
in Ni₃Al and Fe₃Al

Poster

Page: 858

Q. Li, U. Jonas

The evolution of colloidal crystal microstructure during
drying

Poster

Page: 860

X. Xie, X. Li, S. Yan, H. Wu, M. Xu, M. Wang

Properties of ultra-dispersed lithium manganate

Poster

Page: 906

H. Zhiyong, C. Changan, L. Chongxian

Numerical Simulation of Hydrogen Isotopes Diffusion
and Permeation in Stainless Steel

Poster

Page: 910

Symposium 8
Multiscale Simulation Approaches for Static and Dynamic Properties of Macromolecular Materials

Session N

Thursday, 21 September 2006

Location: Lecture hall 1023

Session Chair: K. Kremer

D. N. Theodorou
Hierarchical Modelling of Polymer Physical Properties
9:00 A.M. Page: 947

S. Hyodo
Hierarchical Material Simulation and Coarse Graining
9:40 A.M. Page: 932

K. Jindo, V. V. Hung, N. T. Hoa, M. Menon
Mechanical Properties and Defect Structures of
Nanoscale Materials by Ab Initio Molecular Dynamics
and Temperature Lattice Green's Function Methods
12:40 P.M. Page: 186

Session O

Thursday, 21 September 2006

Location: lecture hall 1023

Session Chair: E. Kaxiras

F. Mueller-Plathe
Challenges in Polymer Simulation
11:00 A.M. Page: 943

T. Uneyama
Mesoscopic Simulation of Micellar Structures in
Amphiphilic Block Copolymer Solutions by the Density
Functional Model
11:40 A.M. Page: 950

G. Goldbeck-Wood, J. Wescott, R. Akkermans, A.
Maiti
Atomistic, Mesoscale and Finite Element techniques
for polymer materials simulations
12:00 P.M. Page: 928

K. Kamio, D. N. Theodorou, K. Moorthi
Multiscale Equilibration of Poly(ethylene terephthalate)
Melt
12:20 P.M. Page: 935

C. Schoen, A. Hannemann, M. Jansen
Modeling the polymer-precursor synthesis of the
amorphous ceramic α -Si₃B₃N₇ via a separation of
time scale stepping stone approach
12:40 P.M. Page: 944

Session P

Thursday, 21 September 2006

Location: lecture hall 1023

Session Chair: D. Theodorou

Lecture hall 1023

B. Duenweg
Computer Simulations of the Dynamics of Polymer
Solutions
2:20 P.M. Page: 921

Effects of hydrodynamic coherence on DNA
translocation: a Lattice Boltzmann-Molecular
Dynamics multiscale approach
3:00 P.M. Page: 939

Y. Masubuchi, G. Ianniruberto, F. Greco, G. Marrucci
Statistics in entangled polymers from primitive chain
network simulations
3:20 P.M. Page: 940

C. Bretthauer, D. Kauzlarić, C. Müller, J. Korvink
Particle based modeling of ultrasonic plastification
with a yield-stress fluid
3:40 P.M. Page: 917

T. Yamaue, Y. Jung, M. Doi
The modeling and simulation of dot formation kinetics
in the drying process of polymer solution drop
4:00 P.M. Page: 953

Poster Session J

Tuesday 19 September 2006, 5:20 P.M. – 8.00 P.M.

Location: Prometheus Hall

and

Poster Session M

Wednesday 20 September 2006, 7:00 P.M. – 9.30
P.M.

Location: Prometheus Hall

N. Arai, K. Yasuoka, Y. Masubuchi
Dissipative Particle Dynamics Simulation for Formation
Process of Threadlike Micelles under Shear Flow
Poster Page: 913

Symposium 9
Materials for Micro-Electro-Mechanical Systems
MEMS

Session P

Thursday, 21 September 2006

Location: lecture hall 1199

Session Chair: J. Korvink

Y. Isono

New Experimental Techniques of Nanofabrication and
Nanomechanics based on MEMS

Lecture hall 1199, 2:20 P.M.

Poster Page: 974

N. Takano

Image-based Multi-scale Simulation of Porous PZT by
Homogenization Theory

Lecture hall 1199, 3.00 P.M.

Poster Page: 981

J. Wilde

Materials-based modelling of non-linear mechanical
MEMS polymers

Lecture hall 1199, 3:40 P.M.

Poster Page: 984

Session S

Friday, 22 September 2006

Location: lecture hall 1199

Session Chair: J. Korvink

V.V.S.D.R. K. Annabattula

Buckle-driven Delamination in Thin Polymer Films

Lecture hall 1199, 10.20 A.M.

Poster Page: 959

P. Berke

Numerical simulation of the nanoindentation
experiment: influence of the experimental
uncertainties

Lecture hall 1199, 10.40 A.M.

Poster Page: 963

J. Gaspar

Strength of LPCVD Silicon Nitride Thin Films

Lecture hall 1199, 11:00 A.M.

Poster Page: 966

Session T

Friday, 22 September 2006

Location: lecture hall 1199

Session Chair: J. Korvink

N. Huber

Modeling and Simulation of Wear in Micro Gears

11:40 A.M. Page: 970

Y. Kang

Experimental Study of Residual Stresses in Nano-
Porous Silicon

12:00 P.M. Page: 978

