

Conference Site:

Veranstaltungszentrum
(Saal 1)
Ruhr-Universität Bochum
44801 Bochum



ADVANCED DISCUSSIONS

Current Developments

26/27 April 2012

Veranstaltungszentrum

Ruhr-Universität Bochum

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RUHR-UNIVERSITÄT BOCHUM



Thursday, 26 April 2012

Light elements and deformation mechanisms

- 9.00 Welcome
- 9.15 Overview
Rebecca Janisch, ICAMS, Thomas Hammerschmidt, ICAMS
- 9.30 Electronic structure method development - Tight-binding models for steel research
Nick Hatcher, ICAMS
- 9.55 Boron in iron and steel - Insights from density-functional theory calculations
Arthur Bialon, ICAMS
- 10.20 Coffee break
- 10.40 Boron added steels - Modern alloying concepts for highstrength steel applications
Andreas Peters, Benteler GmbH
- 11.25 Influence of C on grain boundary cohesion in molybdenum
Arshad Tahir, ICAMS
- 11.50 Analysis of diffusion paths and effective diffusion coefficients in multiphase materials
Philipp Schwittek, ICAMS
- 12.15 Lunch

Kinetics of phase transitions

- 13.30 Overview
Jutta Rogal, ICAMS, Robert Spatschek, MPIE GmbH
- 13.45 Analytic bond-order potentials for simulation of materials properties
Mirek Čák, ICAMS
- 14.20 Computational approaches assisting stress-related design of materials
Petra Sonnweber-Ribic, Robert Bosch GmbH

- 15.00 Coffee break
- 15:30 Modelling of phase change materials with GPUs
Alexander Monas, MPIE GmbH
- 16.05 Large scale phase-field simulations of grain growth
Reza Darvishi, ICAMS
- 16.40 Discussion and closing remarks
- 18.30 Dinner

Friday, 27 April 2012

Thermodynamic modelling

- 9.30 Overview
Suzana Fries, ICAMS, Tilmann Hickel, ASG Modelling, MPIE GmbH
- 9.50 Silicon based thermoelectric materials
Ingo Opahle, ICAMS
- 10.10 Sapiens thermophysical database and software
Mauro Palumbo, ICAMS, Fritz Körmann, ASG Modelling, MPIE GmbH
- 10.30 Coffee break
- 11.00 Discussion on the impact of high additions of Nb in steels
Moderator: Tilmann Hickel, ASG Modelling, MPIE GmbH
An introduction panel will be given by ICAMS/ASG/MPIE researchers and industrial partners on up-to-date experiments, modelling, and industrial demands, followed by an open discussion. Invited speakers are Charles Stallybrass (Salzgitter Mannesmann Forschung), Josef Balun (Benteler GmbH) and Thomas Pretorius (ThyssenKrupp Steel Europe AG)
- 12.20 Conclusions
- 12.30 Lunch
- 14.00 Hands-on course: ICAMS shares its methods