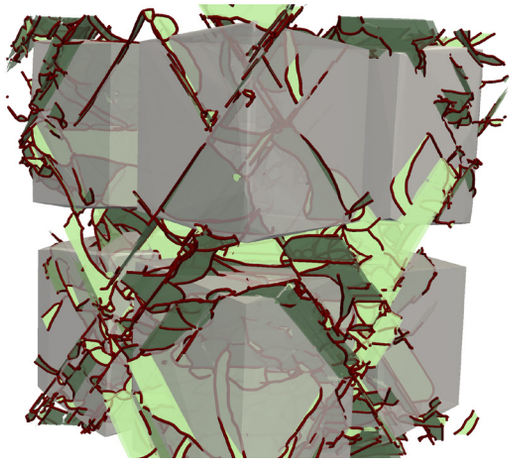
VENUE

WORKSHOP

The workshop will take place in the Conference Centre of the Ruhr-Universität Bochum (room 2b), which is located at the main campus below the mensa. The RUB can be easily reached by public transport. A limited number of parking spaces is available in the nearby P9.

HANDS-ON TUTORIALS AND CLASSES

The tutorials will take place at ICAMS in the building IC in room IC 02/718.



top:
Dislocations cutting the γ-phase during a tensile test
(E. Bitzek, FAU Erlangen)

front:
Stress in the γ/γ' microstructure from large scale atomistic simulations and finite element modelling
(E. Bitzek, J. Amodeo, A. Prakash, FAU Erlangen)

REGISTRATION

- Regular fee: 200 €
- Early bird fee (until July 1): 150 €
- Hands-on tutorials: 80 €

http://www.superalloys.rub.de

ORGANISATION

PROF. DR. RALF DRAUTZ
DR. THOMAS HAMMERSCHMIDT
DR. JUTTA ROGAL

SFB/Transregio 103
SUPERALLOY SINGLE CRYSTALS

Deutsche Forschungsgemeinschaft
DFG

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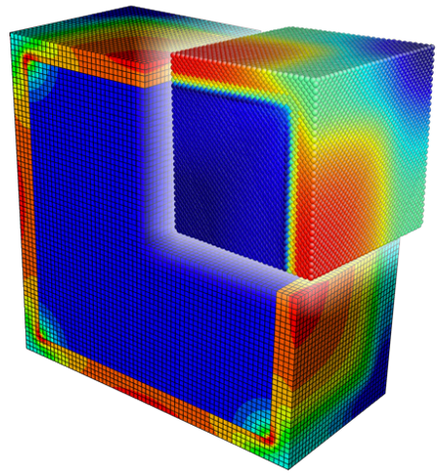
ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

RUB

MODELLING AND SIMULATION OF SUPERALLOYS

INTERNATIONAL WORKSHOP

15-17 September 2014
Bochum, Germany



HANDS-ON TUTORIALS

13+14 September 2014

SFB/Transregio 103
SUPERALLOY SINGLE CRYSTALS

WORKSHOP
15-17 SEPTEMBER 2014

The conference will start on Monday, September 15, 2014 at 1:00 p.m. and will end on Wednesday, September 17, 2014 at 4:00 p.m.

A poster session on Monday evening will give an overview of the research activities of the Collaborative Research Centre SFB/TR 103. Contributed talks and posters of participants are very welcome.
A detailed schedule with session plans can be found on:
http://www.superalloys.rub.de

SCOPE

Superalloys are multi-component materials with complex microstructures that offer unique properties for high-temperature applications. The complexity of the superalloy materials makes it particularly challenging to obtain fundamental insight into their behaviour from the atomic structure to turbine blades. Recent advances in modelling and simulation of superalloys contribute to a better understanding and prediction of materials properties and therefore offer guidance for the development of new alloys.

This workshop will give an overview of recent progress in modelling and simulation of materials for superalloys with a focus on single crystal Ni-base and Co-base alloys. Topics will include electronic structure methods, atomistic simulations, microstructure modelling and modelling of microstructural evolution, solidification and process simulation as well as the modelling of phase stability and thermodynamics.

INVITED SPEAKERS (CONFIRMED)

- **Pyuck-Pa Choi**
  Max Planck Institute for Iron Research, Düsseldorf, Germany
- **Fionn Dunne**
  Imperial College London, London, United Kingdom
- **Nathalie Dupin**
  Calcul Thermodynamique, Orcet, France
- **Gunther Eggeler**
  Ruhr-Universität Bochum, Bochum, Germany
- **Marc Fivel**
  CNRS Institut Polytechnique de Grenoble, St Martin d' Hères, France
- **Alfred Ludwig**
  Ruhr-Universität Bochum, Bochum, Germany
- **Yuri Mishin**
  George Mason University, Fairfax, United States
- **Alessandro Mottura**
  University of Birmingham, Birmingham, United Kingdom
- **Stefan Müller**
  Technische Universität Hamburg-Harburg, Hamburg, Germany
- **Erdmann Spiecker**
  Friedrich-Alexander Universität Erlangen, Erlangen, Germany
- **Anton van der Ven**
  University of California, Santa Barbara, United States
- **Yunzhi Wang**
  Ohio State University, Columbus, United States
- **Chris Wolverton**
  Northwestern University, Evanston, United States

HANDS-ON TUTORIALS AND CLASSES
13+14 SEPTEMBER 2014

Prior to the workshop we offer classes accompanied by hands-on tutorials on modelling and simulation of superalloys. State of the art computational methods ranging from the description of the electronic structure to continuum modelling will be discussed and presented on a level suitable for interested graduate students and postdocs. The number of participants in the tutorials will be limited to 50.

TUTORIALS AND HANDS-ON CLASSES

- Jörg Koßmann, Thomas Hammerschmidt
  Modelling of phase stability with density functional theory
- Sergej Schuwalow, Jutta Rogal
  Diffusion properties from density functional theory
- Juan Wang, Erik Bitzek
  Atomistic simulation of dislocation properties
- Siwen Gao, Anxin Ma
  Discrete dislocation dynamics and crystal plasticity
- Mohan Rajendran, Oleg Shchyglo
  Phase field modelling of precipitation and ripening
- Mauro Palumbo, Suzana Fries
  Thermodynamic modelling using CALPHAD and density functional theory

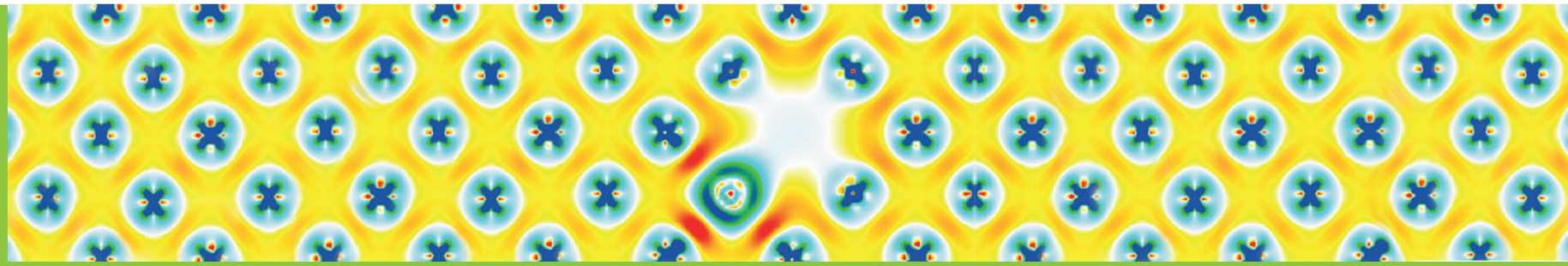


Fig. 1:
Charge density difference plot of a single rhenium atom next to a vacancy in the nickel γ phase.
(S. Schuwalow, ICAMS)