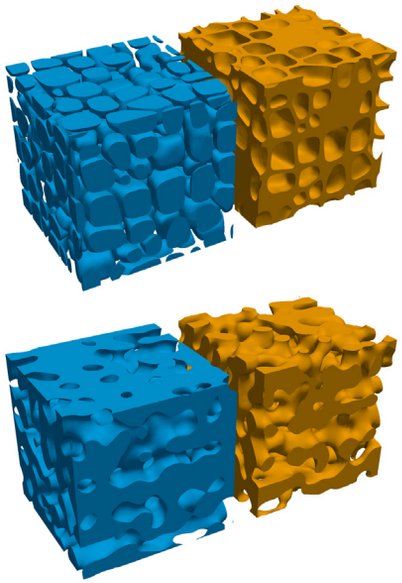
VENUE

WORKSHOP

The workshop will take place at the Conference Centre of the Ruhr-Universität Bochum (room 2b), on 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 parking lot P9.

HANDS-ON TUTORIALS

The hands-on tutorials will take place at ICAMS in building IC in room IC 02/718.



top:
Phase-field simulation of γ/γ' microstructure evolution during long-term aging of Ni-base superalloys.
(Johannes Görler, ICAMS)

front:
Dislocation configuration in the γ/γ' microstructure of Ni-base superalloys.
(Siwen Gao, ICAMS)

back:
Multi-component diffusion channel for solute atoms.
(Sergej Schuwalow, ICAMS)

REGISTRATION

- Workshop fee: 300 €
- Hands-on tutorials: 50 €
  Registration deadline: March 1, 2017

http://www.superalloys2017.rub.de

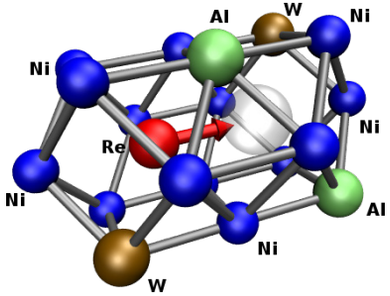
ORGANISATION

RALF DRAUTZ

THOMAS HAMMERSCHMIDT

JUTTA ROGAL

(Ruhr-Universität Bochum)



SFB/Transregio 103
SUPERALLOY SINGLE CRYSTALS

Deutsche Forschungsgemeinschaft
DFG

CONTACT

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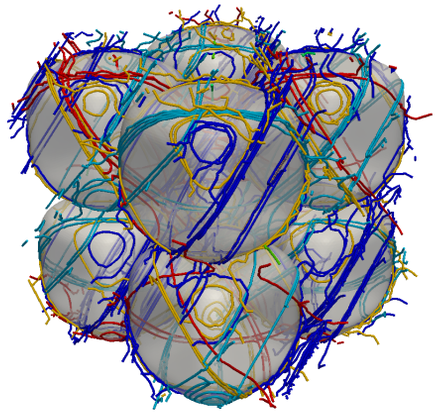
ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

RUB

MODELLING AND SIMULATION OF SUPERALLOYS

INTERNATIONAL WORKSHOP

29-31 March 2017
Bochum, Germany



HANDS-ON TUTORIALS

27+28 March 2017

SFB/Transregio 103
SUPERALLOY SINGLE CRYSTALS

WORKSHOP
29-31 MARCH 2017

The conference will start on Wednesday, March 29, 2017 at 1:00 p.m. and end on Friday, March 31, 2017 at 4:00 p.m.

Contributed talks and posters of participants are welcome. The poster session will take place on Wednesday evening. Posters will also be on display that give an overview of the SFB/TR 103 „From atoms to turbine blades".
A detailed schedule with session plan can be found at:
http://www.superalloys2017.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)

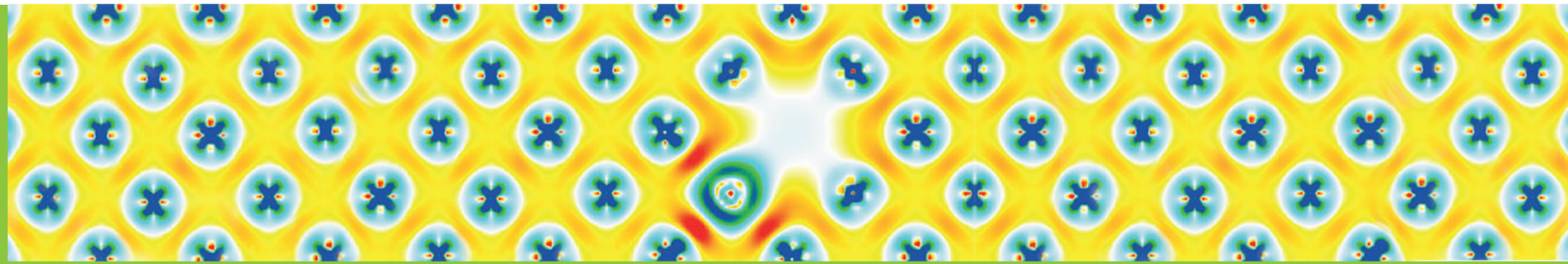
- **Alan Ardell**
  UCLA Engineering, Los Angeles, USA
- **Erik Bitzek**
  Universität Erlangen-Nürnberg, Erlangen, Germany
- **Benoit Devincre**
  CNRS-ONERA, Châtillon Cedex, France
- **Gunther Eggeler**
  Ruhr-Universität Bochum, Bochum, Germany
- **Bernard Fedelich**
  BAM, Berlin, Germany
- **Haruyuki Inui**
  Kyoto University, Kyoto, Japan
- **James Kermode**
  University of Warwick, Coventry, UK
- **Carolin Körner**
  Universität Erlangen-Nürnberg, Erlangen, Germany
- **Catherine Rae**
  University of Cambridge, Cambridge, UK
- **Ralf Rettig**
  Universität Erlangen-Nürnberg, Erlangen, Germany
- **James Saal**
  QuesTek Innovations LLC, Evanston, USA
- **Ingo Steinbach**
  Ruhr-Universität Bochum, Bochum, Germany
- **Dallas Trinkle**
  University of Illinois, Urbana-Champaign, USA
- **Axel van de Walle**
  Brown University, Providence, USA

HANDS-ON TUTORIALS
27+28 MARCH 2017

Prior to the workshop we offer 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 hands-on tutorials will be limited to 50.

HANDS-ON TUTORIALS

- Aparna Puchakayala, Thomas Hammerschmidt
  Phase stability from density functional theory
- Maximilian Grabowski, Jutta Rogal
  Diffusion properties from density functional theory
- Arun Prakash, Frédéric Houllé
  Atomistic simulation of dislocation properties
- Siwen Gao
  Discrete dislocation dynamics and crystal plasticity
- Johannes Görler, Oleg Shchyglo
  Phase field modelling of precipitation and ripening
- Helge Schaar, Suzana Fries
  Thermodynamic modelling using CALPHAD



Charge density difference plot of a single rhenium atom next to a vacancy in nickel. (Sergej Schuwalow, ICAMS)