Expert Committee Materials Modelling, Simulation and Data

Place: Room "Lennep", 1. OG, Technologiezentrum am Europaplatz (TZA)
Dennewartstraße 25-27, 52068 Aachen

& Online

Date: 17 - 18 April 2023

Agenda

Monday, 17 April 2023

14:00 Arrival in Aachen / Online login / Welcome and Introduction
S. Sandfeld, Forschungszentrum Jülich

Working Group „3D Material Data“
S. Sandfeld, Forschungszentrum Jülich

14:10 Materials informatics for plasticity
Stricker, M. (Speaker)[1]
[1]Ruhr-Universität Bochum (RUB)

14:30 *ONLINE*
Data-based modelling of the structural stability of intermetallics
Hammerschmidt, T. (Speaker)[1]
[1]Ruhr-Universität Bochum (RUB)

14:50 Social Networking and graph mining in material science for the prediction of material properties
Jalali, M. (Speaker)[1]
[1]Karlsruhe Institute of Technology (KIT)

15:10 Break and Postershow

Working Group “Simulation Platform and Interoperability”
D. Höche, Helmholtz-Zentrum Hereon; M. Apel, ACCESS e.V.

15:40 Update to the Plattform Material Digital
Hickel, T. (Speaker)[1]
[1]Max-Planck-Institut für Eisenforschung GmbH

16:00 Digital Thread for manufacturing towards improved part quality and quicker process qualification
Megahed, M. (Speaker)[1]
[1]ESI Group

16:20 *ONLINE*
preCICE – A General-Purpose Simulation Coupling Interface
Ueckermann, B. (Speaker)[1]
[1]University of Stuttgart

16:40 Break and Postershow

Working Group „Atomistic“
T. Hickel, MPI für Eisenforschung GmbH; R. Janisch, RUB; E. Bitzek, MPI für Eisenforschung

17:10 *ONLINE*
Modelling mechanochemical reactions in epoxy resins using hybrid QM/MM/MD approaches
Wick, C.R.[1]
[1]Friedrich-Alexander-Universität Erlangen-Nürnberg

17:30 Machine Learning Interatomic Potentials: Why we need them and how to train them
Poul, M.[1]
[1]Max-Planck Institut für Eisenforschung Düsseldorf

17:50 *ONLINE*
Understanding orientation and strain partitioning in atomistic simulations via statistical machine learning
Prakash, A.[1]
[1]TU Bergakademie Freiberg

18:10 End

19:00 Meeting in the KOCHKULTUR" Passstr. 79 (cost prize base)

Tuesday, 18 April 2023

Working Group „Microstructural Mechanics“
A. Hartmaier, Ruhr-Universität Bochum; S. Klinge, TU Berlin

09:00 Multiscale Modeling of Calcified Polymer Hydrogels
Klinge, S. (Speaker)[1]; Graham, M.[1]
[1]TU Berlin

09:20 Material parameter determination from ab-initio data for two-dimensional materials
Shirazian, F. (Speaker)[1]; Sauer, R.A.[1]
[1]RWTH Aachen University

09:40 Development of a framework for load case dependent microstructure design
Henrich, M. (Speaker)[1]; Fehlemann, N.[1]; Münstermann, S.[1]
[1]RWTH Aachen University

10:00 Break and Postershow

Working Group „Phase Field Modelling"
Britta Nestler, Daniel Schneider, KIT Karlsruhe

10:30 Crack propagation phase-field modeling considering for multi-crack order parameters and mechanical jump
Schöller, L. (Speaker)[1]; Schneider, D.[2]; Prahs, A.[2]; Nestler, B.[2]
[1]Karlsruhe University of Applied Sciences; [2]Karlsruhe Institute of Technology (KIT)

10:50 Comparative assessment of adaptive spatial refinement strategies in 3D phase-field fracture simulations of brittle materials
Rohracker, M. (Speaker)[1]; Mergheim, J.[1]
[1]Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

11:10 Modular phase-field modeling of fatigue crack initiation and growth: Application to gear failure mode tooth flank fracture
Schneider, T. (Speaker)[1]; Müller, D.[2]; Kalina, M.[1]; Tobie, T.[2]; Stahl, K.[2]; Kästner, M.[1]
[1]TU Dresden; [2]Technical University of Munich

11:30 Wrap up

12:00 End of the meeting

Poster-Presentations:

Ontologies for defects in crystals and computational samples
Azocar Guzman, A. (Speaker)[1]; Menon, S.[2]; Hofmann, V.[1]; Hickel, T.[2]; Sandfeld, S.[1]
[1]Forschungszentrum Jülich GmbH, Aachen; [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Atomistic phase stability data at 0 K --> Calphad databases --> high-throughput Calphad calculations
to Baben, M. (Speaker)[1]
[1]GTT-Technologies, Herzogenrath

Dislocation-mediated plasticity in the SmCo5 phase
Stollenwerk, T.[1]; Ulumuddin, N. (Speaker)[1]; Sun, P.-L.[1]; Lee, S.-H.[1]; Seehaus, M.[1]; Skokov, K.[2]; Gutfleisch, O.[2]; Xie, Z.[1]; Korte-Kerzel, S.[1]
[1]RWTH Aachen University; [2]TU Darmstadt

Phase-field-model simulation of abnormal/normal recrystallization kinetics in ultrafine-grained aluminum processed by high pressure torsion extrusion
Abramova, O. (Speaker)[1]; Schneider, D. (Speaker)[1]; Baretzky, B.[1]; Ivanisenko, J.[1]; Nestler, B.[1]; Nugmanov, D.[1]; Prahs, A.[1]
[1]Karlsruhe Institute of Technology (KIT)

ALAMEL/VEF
Schildermans, S. (Speaker)[1]
[1]KU Leuven

3D full-field crystal plasticity simulations on an explicit microstructure: How accurate are we?
Prabhu, N. (Speaker)[1]; Diehl, M.[1]
[1]KU Leuven

Assessment of semi-empirical potentials of Mg and its alloys
Wang, H. (Speaker)[1]; Guénolé, J.[2]; Korte-Kerzel, S.[1]; Al-Samman, T.[1]; Xie, Z.[1]
[1]RWTH Aachen University; [2]Université de Lorraine, CNRS, Arts et Métiers, Metz (France)

Unveiling the mechanisms of plastic deformation in Laves crystals
Xie, Z. (Speaker)[1]; Atila, A.[2]; Bitzek, E.[3]; Chauraud, D.[3]; Guénolé, J.[4]; Korte-Kerzel, S.[1]; Luo, W.[1]; Pizzagalli, L.[5]
[1]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University; [2]Lehrstuhl für Materialsimulation, Universität des Saarlandes, Saarbrücken; [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf; [4]Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, Metz (France); [5]Institut P', CNRS UPR 3346, Université de Poitiers, SP2MI

Lecture time: 20 minutes (15 min. talk + 5 min. discussion)
Poster will be discussed during the breaks

Please register under this link for the meeting

All persons who have registered for online participation will receive the access link by email a few days before the meeting.