 # 24 Poster 2023-04-10 23:08:11

3D Materials Data

3D full-field crystal plasticity simulations on an explicit microstructure: How accurate are we?

Prabhu, N. (Speaker)[1]; Diehl, M.[1]

[1]KU Leuven

With advancements in material characterization techniques, material scientists aiming to model micro-mechanical behavior now have copious data at their disposal. How they can effectually utilize this abundant data remains the central question. The dataset of interest for this study was provided as a part of challenge 4 of the Air Force Research Laboratory (AFRL) Additive Manufacturing (AM) modeling challenge series. Precisely, the grain-averaged initial elastic strain data for a distinct set of grains in an AM Inconel 625 alloy alongside specimen's explicit 3D microstructure image data. In-situ data acquisition during the uniaxial tensile test allowed to extract elastic strains of the aforementioned set of grains during six additional load states. This work aimed to incorporate the initial elastic strain data in our full-field crystal plasticity simulations and assess model performance by juxtaposing experimental and simulated elastic strains for the subsequent load states along the tensile test.

 # 17 Poster 2023-04-05 16:11:16

Atomistic

Atomistic phase stability data at 0 K --> Calphad databases --> high-throughput Calphad calculations

to Baben, M. (Speaker)[1]

[1]GTT-Technologies, Herzogenrath

The poster will demonstrate the whole workflow from atomistic phase stability data to Calphad databases and then to high-throughput Calphad calculations for materials design.

Step 1: How 0 K phase stability data data is extrapolated to technically relevant temperatures based on ML models using features from atomistic simulation data but experimentally-based training data. This is done for all compounds in Materials Project [1] and in OQMD [2] and was used to develop the Calphad databases aiMP and aiOQ [3].

Step 2: How Calphad databases can be used for high-throughput Calphad calculations in materials design efforts. Here, three examples will be highlighted: a) The search of whole periodic table of elements to identify coating materials for SiC/SiC composites to improve high-temperature oxidation resistance both under air and steam atmosphere. b) The search of a 12-component chemical space to identify cheap hard-facing alloys for mining applications. c) The search of a six-component salt system to identify eutectics that can serve as heat storage materials.

[1]: Jain et al., APL Materials, 1 (2013) 011002.

[2]: Saal et al., JOM 65 (2013) 1501.

[3]: https://gtt-technologies.de/data/#aimp-ab-initio-materials-project

 # 18 Poster 2023-04-06 13:05:39

Atomistic

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)

Atomistic simulation using classical semi-empirical potentials is an important way to gain insight into the microscopic deformation mechanisms, particularly interactions of crystallographic defects in materials. However, the selection of inappropriate potentials can lead to uncertainties in the observed mechanisms due to the artefacts associated with them. Therefore, a systematic assessment of the relevant interatomic potentials for a particular material system is essential. In the present study, we systematically evaluated interatomic potentials of Mg and its alloys, including embedded-atom method (EAM) and modified embedded-atom method (MEAM) potentials, by means of different material characteristics, such as elastic properties, stacking fault energies, grain boundary (GB) energies, per-site segregation energies, as well as dislocation motion on basal, prismatic, and pyramidal planes. The results are compared with experiments and density functional theory (DFT) calculations from the literatures. We found that the EAM potentials, although more efficient for modeling fundamental properties, differed significantly from experimental observations in describing dislocation properties. In addition, we found a strong correlation between the per-site segregation energies of alloying elements at GBs and the local GB site volumes.

 # 23 Poster 2023-04-10 10:26:55

Atomistic

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

Laves phases are topologically close-packed structures that form in many alloys and serve as fundamental building blocks in complex intermetallics. A thorough comprehension of the plasticity in Laves crystals would facilitate knowledge transfer to numerous complex phases and composites. In this study, the mechanisms of motion of synchro-Shockley dislocations were investigated using atomistic simulations. We demonstrated the thermally activated nature of synchro-Shockley dislocations, providing insight into the atomic origin of room-temperature brittleness in Laves phases. We explored how vacancies and antisite defects assist kink nucleation and propagation, which are crucial for dislocation mobility in such material. Furthermore, using ab initio calculations, we revealed the effects of structure and composition on the mechanical properties and deformation mechanisms of Laves and μ phases. Our findings shed light on how temperature and chemical composition affect the plastic deformation induced by zonal dislocations in Laves phases and provide avenues for tailoring the mechanical properties of complex intermetallics.

 # 20 Poster 2023-04-06 17:21:30

Microstructural mechanics

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

Research on the mechanical properties of complex intermetallics is relatively scarce. It is hypothesized that complex phases, such as Sm_2Co_7, will exhibit deformation behavior that is a combination of the structural properties of their underlying building block phases, which in this case are $SmCo_5$ and $SmCo_2$. In this work, the deformation behavior of $SmCo_5$ was investigated through the nanoindentation and micropillar compression of its single crystals. The basal (0001) [2$\bar{1}\bar{1}$0], pyramidal II (2 $\bar{1}$ $\bar{1}$ $\bar{1}$) [$\bar{2}$ 1 1 $\bar{6}$] and pyramidal I (0 $\bar{1}$ 1 1) [2 $\bar{1}$ $\bar{1}$ 0] slip systems were observed experimentally. Density functional theory and molecular statics were then used to rationalize and provide insights into the nature of these slip systems. The calculations demonstrated the orientation dependence of stacking fault formation on the basal (0 0 0 1) slip system, the existence of multiple partial dislocations on the pyramidal II (2 $\bar{1}$ $\bar{1}$ $\bar{1}$) plane, as well as the non-crystallographic nature of the pyramidal I (0 $\bar{1}$ 1 1) slip system. This work suggests that plasticity is enabled through dislocation-mediated deformation mechanisms, which contrasts with earlier claims that amorphous shear bands are the primary drivers of plasticity in $SmCo_5$. Our findings thus serve as a basis to understand the deformation behavior of structurally related phases in the Sm-Co system.

 # 9 Lecture 2023-03-13 10:07:47

Microstructural mechanics

Multiscale Modeling of Calcified Polymer Hydrogels

Klinge, S. (Speaker)[1]; Graham, M.[1]

[1]TU Berlin

Hydrogels, a significant group of highly hydrated polymers, represent the best choice for the potential application to bone fracture regeneration, which goes back to their bioactivity, affinity for biologically active proteins and compatibility with the bone tissue. However, this kind of materials also shows a serious disadvantage, namely, it loses its mechanical strength through swelling. This makes its straightforward usage difficult and motivates the development of different enhancement procedures. One of the most modern techniques for this purpose is calcification or, in a more general sense, mineralization. This method is inspired by the natural process of the bone growth where the enzyme alkaline phosphatase causes mineralization of the bone by cleavage of the phosphate from organic molecules. An analogous process induces homogeneous mineralization of a hydrogel and increases its mechanical strength. Recently, optical and electron microscopy has revealed that calcification yields different types of microstructure dependent on the type of the underlying polymer, and thus has clearly indicated that computational modeling can significantly contribute to the targeted investigation of effective behavior and material parameters. The current contribution uses the multiscale finite element method to simulate the effective material behavior of calcified hydrogels. Within this framework, representative volume elements (RVEs) are generated to depict the biphasic material microstructure consisting of the organic hydrogel and anorganic calcium phosphate. Most commonly, the anorganic phase appears in the form of spherical inclusions or honeycomb grids where the characteristic size of a typical unit might vary. The approach proposed treats the calcified regions as linear elastic material and assumes the Ogden model for the hydrogel. Diffusivity is another important aspect in this context. Its study requires a profound knowledge on the processes on the nanoscale. This time, the effective behavior is investigated by using the asymptotic homogenization approach.

[1] S. Aygün and S. Klinge, Two-Scale Computational Homogenization of Calcified Hydrogels. Math. Meth. Appl. Sci. 2023.

 # 7 Lecture 2023-03-02 14:44:18

Microstructural mechanics

Development of a framework for load case dependent microstructure design

Henrich, M. (Speaker)[1]; Fehlemann, N.[1]; Münstermann, S.[1]

[1]RWTH Aachen University

In this talk a framework for microstructure design under arbitrary loading conditions, using RVEs and crystal plasticity simulations will be presented. The RVE-generator developed by our team uses deep learning and discrete grids to reconstruct complex morphologies of steel microstructures. The generator is used for microstructural design using a Bayesian optimization approach. The proposed approach is demonstrated on a dual phases steel considering different load cases.

 # 19 Poster 2023-04-06 15:48:23

Phase Field Modelling

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)

The digital twin of the recrystallization (ReX) kinetics in pure Al subjected to severe plastic deformation by High Pressure Torsion Extrusion was created in the PACE2D using the phase-field model (PFM). Experimental investigation of the ReX kinetics at 300°C of pure Al after HPTE v1ω1 regime was carried out. The as-deformed structure of Al was implemented for the ReX simulation by PFM. The simulated ReX kinetics demonstrates, that the bimodal distributions of the (sub)grain size are formed, in agreement with the experiment. Furthermore the PFM calculation demonstrates a transition of the ReX kinetics from a normal grain growth to the abnormal one, NGG and AGG without separation of grains into fractions with different grain growth rates. Analysis of the simulated microstructures allows to extract the criteria for the development of the NGG and AGG.

 # 1 Lecture 2023-02-23 12:02:07

Phase Field Modelling

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)

In current material science, the phase field method is widely used to model fracture propagation since it enables implicit tracking of the crack surface. Further, they show good agreement with analytical solutions and are capable of describing complex fracture behavior. Nevertheless, most of these crack propagation models have been introduced for homogeneous materials, and there only exist a few approaches for heterogeneous systems. However, these approaches have some limitations, as recently discussed by Henry [2] and Schöller et al. [3] as they may yield unphysical fracture behavior. So models, that are able to describe the crack propagation in such systems, are highly desirable. Therefore, models that can describe crack propagation qualitatively in such systems are highly desirable. A novel approach, introduces multiple crack order parameters, tracking only the damage of a corresponding subregion [3]. This new approach is compared with a classical phase-field approach to crack propagation that uses interpolated crack surface energies. Therefore, a crack propagating along a sloped material interface is utilized to demonstrate the qualitative and quantitative differences between both models. The results are compared to an analytical solution based on linear elastic fracture mechanics. Subsequently the new model is applied to fiber-reinforced polymers and is able to predict fracture in heterogeneous two phase systems. Furthermore the underlying homogenization problem for the elastic material properties is discussed. The limitations of the basic linear interpolation scheme are shown, since contrary contrasts of elastic modulus and crack resistance can lead to unreasonable crack paths. The consideration of mechanical jump condition [1] yields phase-specific stresses and strains. Based on this the mechanical driving force for the crack propagation can be modeled as more independent of the elastic properties than of other physical regions. Thus taking into account the mechanical jump conditions instead yields still reasonable results, whereas the simple scheme fails to predict the fracture behavior [4].

[1] D. Schneider, F. Schwab, E. Schoof, A. Reiter, C. Herrmann, M. Selzer, T. Böhlke, and B. Nestler, 2017 On the stress calculation within phase-field approaches: a model for finite deformations. Computational Mechanics, 60(2), 203–217.
[2] H. Henry, 2019 Limitations of the modelling of crack propagating through heterogeneous material using a phase field approach. Theoretical and Applied Fracture Mechanics, 104, 102384.
[3] L. Schöller, D. Schneider, C. Herrmann, A. Prahs, and B. Nestler, 2022, Phase-field modeling of crack propagation in heterogeneous materials with multiple crack order parameters. Comp. Meth. App. Mech. Eng., 395, 114965.

 # 2 Lecture 2023-02-23 14:56:00

Phase Field Modelling

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)

Phase-field fracture simulations of brittle materials have gained enormous interest in recent years. Here, the smeared phase-field function approximates the discrete crack. For a proper resolution of the phase-field function, suitable meshes in regions of the expected crack propagation are required. Pre-refining the mesh in the anticipated crack propagation region fulfills this requirement. However, this could lead to simulations of high computational costs due to many elements. An alternative option is to utilize adaptive spatial refinement (ASR) strategies based on appropriate error indicators. We expand our previous work (cf. [1]) by the three-dimensional comparison of different error indicators used for ASR in the simulation of the single edge notch shear (SENS) test. Here, three distinct criteria are analyzed, the phase- field threshold, the Kelly error indicator, and the newly derived configurational force-based error indicator. The performance of the three different ASR strategies is compared through the speedup and their accuracy through a relative error in correlation to a reference simulation obtained on a pre-refined mesh.

[1] M. Rohracker, P. Kumar, and J. Mergheim, 2023, A comparative assessment of different adaptive spatial refinement strategies in phase-field fracture models for brittle fracture. Forces in Mechanics, 100157.

 # 3 Lecture 2023-02-26 17:06:06

Phase Field Modelling

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

Tooth flank fracture (TFF) is a fatigue failure mode in gears in which the crack is initiated within the tooth volume. Hertzian contact loads in combination with case-hardening induced residual stresses and inhomogeneous material properties lead to crack initiation sites in larger material depth and crack growth invisible from the outside. Recently, for modeling crack growth and even fatigue crack growth efficiently within a finite element model, the phase-field method has gained popularity. We present a numerical approach [1] to model the initiation and growth of subsurface fatigue cracks during TFF. Therefore, a phase-field model for fatigue fracture [2] is revisited and extended in a modular way to account for rolling contact multiaxial high cycle fatigue. Fatigue effects are introduced to the phase-field by using a local lifetime variable for lowering the model's fracture toughness gradually. For this purpose, the dang van critical plane approach is applied to account for rolling contact fatigue present during gear meshing. In the modeling of the meshing process, a simplified approach is used to allow an efficient simulation. We show the implementation of a 2D finite-element gear tooth model explicitly incorporating inhomogeneous material properties and residual stresses, which are considered for both the phase-field crack driving force and the calculation of the local lifetime variable. Numerical results are compared to experimental investigations on crack initiation and growth during TFF in a test gearing. Thereby, special focus is put on the ability of the proposed model to reproduce the experimentally observable subsurface cracking behavior. The numerical results are promising since the typical crack initiation and crack path of TFF are predicted well.

References

[1] T. Schneider, D. Müller, M. Seiler, T. Tobie, K. Stahl and M. Kästner, 2022, Phase-field modeling of fatigue
crack growth during tooth flank fracture in case-hardened spur gears. Int. J. Fatigue 163, p. 107091.

[2] M. Seiler, T. Linse, P. Hantschke and M. Kästner, 2020, An efficient phase-field model for fatigue fracture in
ductile materials Eng. Frac. Mech. 224, p. 106807.

 # 21 Poster 2023-04-06 17:25:44

Simulation Platform and Interoperability

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

The microstructures of materials are characterized by defects, which determine the materials performance. To evaluate them, researchers working on atomistic simulations often perform calculations with different codes (e.g., in scale-bridging approaches). In such cases, it is beneficial to reuse existing atomic structures (samples). To aid the reuse of these computational samples, well-described and harmonized metadata and data is crucial, however, most standardization approaches are focused only on perfect crystal structures, and not on defects. The description of defects and application level information of atomic samples is needed. Another challenge is that file formats used for crystallographic structures (which are often specifically tailored to a certain code) have different representations, which can lead to difficulties transitioning between codes and information being dropped. Finally, another issue preventing the reusability of atomic structure samples is the lack of information on the creation workflow or provenance.

We develop an application-level ontology for material science computational samples, CMSO, which initially describes samples on the atomistic level. The use of this ontology is aided by a software tool for automated annotation of structures using available atomic structural codes. Pyscal-rdf provides a way for users of common atomistic structure codes to implement RDF store and SPARQL querying. The use of this controlled vocabulary in a linked open data form ensures interoperability between different structural file formats and software, while also offering the possibility of making data findable and reusable.

 # 5 Lecture

Simulation Platform and Interoperability

Plattform MaterialDigital: Status and recent developments

Hickel, T. (Speaker)[1]

[1]Max-Planck-Institut für Eisenforschung GmbH

The “Innovation Platform MaterialDigital" (PMD) funded by the German Federal Ministry of Education and Research (BMBF), aims to develop a sustainable infrastructure for the standardized digital representation of materials science and materials engineering. With its partners (KIT, Fraunhofer IWM, FIZ, Leibnitz IWT, BAM, MPIE), the PMD is committed to build up a materials science data space. To achieve this the PMD provides a prototypical infrastructure for the digitalization of materials implemented by decentralized data servers, standardized data schemas and digital workflows. Standards, methods, and tools developed within the platform are deployed and consolidated within the context of BMBF-funded academic and industrial research projects and made available to the material science community in general. In this context scientific workflows represent a major focus area, represented within the platform by the workflow frameworks pyiron and SimStack. In consequence, the platform is building up a digital library in form of a workflow store along with common standards for the definition and representation of digital workflows. We present the activities within the PMD with a particular focus on the workflow group. The current status and the vision for a dissemination of the solutions developed in the PMD within the community are provided.

 # 4 Lecture

Simulation Platform and Interoperability

Digital Thread for manufacturing towards improved part quality and quicker process qualification

Megahed, M. (Speaker)[1]

[1]ESI Group

Modelling material processing and product performance necessitate the use of a unified ontology and flexible data structures to ensure interoperability of the simulation tools and seamless transfer of data across length and time scales. A digital thread based on AutomationML is introduced that combines both physics- and data-based modelling. The digital platform combines off-line simulation tools, the results of which are utilized in data-bases and/or as reduced order models for in-situ control of the process. Optimization loops and decision support prior to manufacturing the component are supported. Online monitors can reference the expected behavior to flag issues during manufacturing. Deviations from the designed process initiate corrective measures that are documented for later reference and use.

This presentation will show different aspects of the digital thread using Laser Metal Deposition (LMD) and associated preprocessing, inspection and quality assurance for a scaled down aerospace engine casing as a demonstrator.

 # 22 Poster 2023-04-07 14:04:21

Simulation Platform and Interoperability

ALAMEL/VEF

Schildermans, S. (Speaker)[1]

[1]KU Leuven

ALAMEL/VEF is a versatile crystal plasticity modeling framework with the excellent performance of Taylor-type models but with improved accuracy. The tool is aimed at industry and supports a variety of constitutive models as well as stress- and strain-driven simulations.

 # 6 Lecture

Simulation Platform and Interoperability

preCICE – A General-Purpose Simulation Coupling Interface

Ueckermann, B. (Speaker)[1]

[1]University of Stuttgart

preCICE (https://precice.org/) is an open-source coupling software for partitioned multi-physics and multi-scale simulations. Thanks to the software's library approach (the simulations call the coupling) and its high-level API, only minimally-invasive changes are required to prepare an existing (legacy) simulation software for coupling. Moreover, ready-to-use adapters for many popular simulation software packages are available, e.g. for OpenFOAM, SU2, CalculiX, FEniCS, and deal.II. For the actual coupling, preCICE offers methods for fixed-point acceleration (quasi-Newton acceleration), fully parallel communication (MPI or TCP/IP), data mapping (radial-basis function interpolation), and time interpolation (waveform relaxation). Today, although being an academic software project at heart, preCICE is used by more than 100 research groups in both academia and industry.

 # 11 Lecture

Materials informatics for plasticity

Stricker, M.[1]

[1]Ruhr-Universität Bochum

 # 13 Lecture

Social Networking and graph mining in material science for the prediction of material properties

Jalali, M. (Speaker)[1]

[1]Karlsruhe Institute of Technology (KIT)

 # 12 Lecture

Data-based modelling of the structural stability of intermetallics

Hammerschmidt, T. (Speaker)[1]

[1]Ruhr-Universität Bochum

 # 15 Lecture

Machine Learning Interatomic Potentials: Why we need them and how to train them

Poul, M. (Speaker)[1]

[1]Max-Planck-Institut für Eisenforschung GmbH

 # 16 Lecture

Understanding orientation and strain partitioning in atomistic simulations via statistical machine learning

Prakash, A. (Speaker)[1]

[1]TU Bergakademie Freiberg

[4] L. Schöller, D. Schneider, C. Herrmann, A. Prahs, and B. Nestler, 2022, Phase-field modeling of crack propagation based on multi-crack order parameters considering mechanical jump conditions. PAMM, accepted.