TECHNISCHE UNIVERSITÄT DRESDEN

DCMS MATERIALS 4.0 SUMMER SCHOOL

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DEEP MECHANICS

#materials40

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DRESDEN concept
Exzellenz aus Wissenschaft und Kultur

WELCOME

Innovative materials are one of the key technologies for keeping products and industrial processes economically competitive and ecologically sustainable. Modern materials science requires a multi-discipline approach embracing chemistry, physics, engineering, as well as theoretical and numerical modelling. The DCMS MATERIALS 4.0 summer school ***Deep Mechanics*** will provide an overview of current developments in the ongoing digitalisation revolution in materials science and will offer a platform for discussions about future perspectives. The summer school targets **Master students**, **PhD students** and (early-stage) **Postdocs**.

This summer school is part of TU Dresden's Institutional Strategy, funded by the Excellence Initiative of the German Federal and State Governments. The school receives additional funding through the Helmholtz Excellence Network DCM-MatDNA.

SCIENTIFIC ORGANIZATION

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TU Dresden

Prof. Sibylle Gemming
HZDR and
TU Chemnitz

Prof. Markus Kästner
TU Dresden

ORGANIZING BOARD

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LOCATIONS

TU DRESDEN CAMPUS

The Technische Universität Dresden (TUD) is one of the largest "Technische Universitäten" in Germany and one of the leading and most dynamic universities in Germany. As a full-curriculum university with 18 faculties in five schools it offers a broad variety of 121 disciplines and covers a wide research spectrum. Its focuses of Biomedicine, Bioengineering, Materials sciences, Information technology, Microelectronics as well as Energy and Environment are considered exemplary in Germany and throughout Europe. About 34.000 students are enrolled at TUD - about one eighths of its students come from abroad. Since 2012, the TUD is one of the eleven Excellence Initiative universities in Germany.

The summer school will take place in the **Görges building GÖR 229** (Helmholtzstr. 9, 01069 Dresden, see also https://goo.gl/maps/pzmjLwGNe1GGEBNcA)**,** which is located on the main campus of TUD.

HOW TO GET THERE

From **Postplatz** you can take tram line **11 (Zschertnitz)** and change at **Walpurgisstraße** to tram line **3 (Coschütz)**. Leaving the tram at **Münchner Platz** will allow you to easily reach the summer school venue.

IBIS BUDGET HOTEL DRESDEN CITY

This contemporary hotel, next to the Altmarkt-Galerie shopping mall, is a 6-minute walk from the Zwinger museum complex and 1.3 km from the Dresden train station. The hotel room can be entered on the day of arrival at 14:00 at the earliest and is available until the day of departure 12:00 at the latest.

PROGRAM

	19-Aug-19	20-Aug-19	21-Aug-19	22-Aug-19	23-Aug-19
	Monday	**Tuesday**	**Wednesday**	**Thursday**	**Friday**
09:00-09:30	registration	Stefanie Reese (RWTH)	Daniel Urban (FhG IWM)	Benjamin Klusemann (HZ Geesthacht)	Anja Waske (BAM)
09:30-10:00	welcome & opening				
10:00-10:30			Weihui Xie (SJTU)		Amber Geurts (Aalto)
10:30-11:00	Federico Zipoli (IBM Zurich)	coffee break	coffee break / luncheon	coffee break	
11:00-11:30		Patrick Rinke (Aalto)		Rebecca Janisch (RUB)	coffee break
11:30-12:00	luncheon		excursion to *VW Gläserne Manufaktur* and cultural program		Surya Kalidindi (Georgia Tech)
12:00-12:30					
12:30-13:00		luncheon		luncheon	luncheon
13:00-13:30	Thomas Lehmann (TU Dresden)				
13:30-14:00		Frank & Holger Großmann (SAP & Anton Paar)			
14:00-14:30				Marc-Andre Keip (U Stuttgart)	round table with participants
14:30-15:00		Emre Topal (FhG IKTS)			
15:00-15:30	coffee break				
15:30-16:00	Thomas Lehmann (TU Dresden)	coffee break		coffee break	closing
16:00-16:30		lab visits and art exhibition		Felix Göküzüm (U Stuttgart)	
16:30-17:00					
17:00-17:30	get-to-know	contributed talks and poster session I		contributed talks and poster session II	
17:30-18:00					
18:00-19:00					
19:00-20:00					
20:00-20:30					

Keynote Lectures	
Federico Zipoli	Accelerated Material Discovery
Surya R. Kalidindi	Materials Innovation Driven by Data and Knowledge Systems

Lectures	
Amber Geurts	From margins to mainstream: the emergence of data- driven materials research as field of science and business
Felix Gökküzüm	On the use of machine learning methods in multiscale modeling: Hands-on session
Frank & Holger Großmann	Materials 4.0 can only exist with blockchain solutions
Rebecca Janisch	Atomistic aspects of deformation and fracture
Marc-Andre Keip	On the use of machine learning methods in multiscale modeling
Benjamin Klusemann	Application of machine learning approaches in the context of processes and materials with focus on artificial neural networks
Thomas Lehmann	Machine Learning with Python: Hands-on session
Stefanie Reese	Model reduction and data-driven mechanics - developments and applications
Patrick Rinke	Machine Learning in Materials Science
Emre Topal	Neuronal Networks for the improved reconstruction of X-ray CT Data
Daniel Urban	Building a materials database for the digital representation and modelling of materials along the product life cycle
Anja Waske	Non-destructive testing of materials and composites
Weihui Xie	SJTU and Zhi-hong Summer School Series

Contributed Talks	
Omur E. Dagdeviren	Controlled Manipulation of Individual Molecules on Surfaces and Comparison with Machine Learning Approaches
Robert Jones	Plasmonic Nanocatalysis - Do shape and size matter?
Guohua Zhao	Understanding alloy compositions and strain-hardening of TWIP Ti alloys: Material informatics and dislocation-based modelling
Ahmad Zainul Ihsan	Data Mining of Dislocation Microstructures: Approximating Dislocation Curvature

Deep Materials:
Perspectives on data-driven materials research

Monday, Aug 19th 2019 – Friday, Aug 23th 2019

Dresden | Germany

BOOK OF ABSTRACTS

This summer school is part of TU Dresden's Institutional Strategy, funded by the Excellence Initiative of the German Federal and State Governments. The school receives additional funding through the Helmholtz Excellence Network DCM-MatDNA.

CONTENT

LECTURES

CONTRIBUTED TALKS AND POSTERS

POSTERS

DCMS
MATERIALS 4.0
SUMMER SCHOOL

LECTURES

FEDERICO ZIPOLI

IBM Zurich, Switzerland
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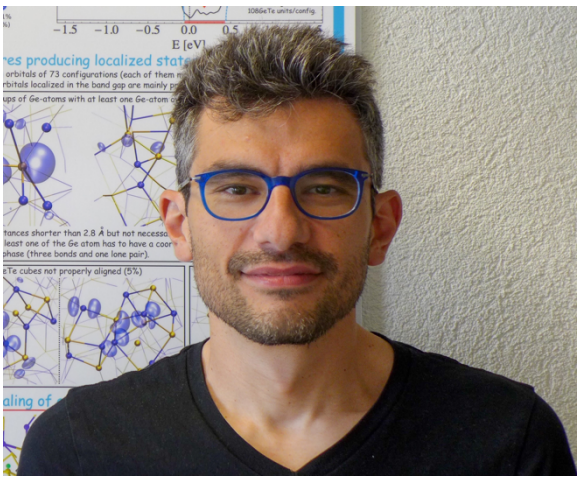
Accelerated Material Discovery

Experiments and theory have been widely used to drive the discovery novel material. In the last decades, also simulations contributed to speed up innovation. *In silico* experiments became the third pillar of research. Today, the scientific community produces continuously a large amount of data which are made available via publications. It is becoming difficult for a researcher to follow such stream of information. Many researchers believe that data are becoming the fourth pillar of research. If we could efficiently consume data, we could face a disruptive opportunity of accelerating innovation. The work I will present is focused on extracting information from different unstructured sources with the goal of building a platform which can allow a researcher, expert in the field, to efficiently retrieve and link facts. Our current work is focused on building a platform that can connect data from different sources to allow inference and analytics to drive new discovery.

In my presentation, I will illustrate our team effort at IBM Research – Zurich to develop the building blocks which can enable such platform. In particular, I will focus on data ingestion from PDF documents and extracting information from text, tables, images with the goal of building a knowledge graph suitable for Q&A.

Biography



Dr. Federico Zipoli is a Research Staff Member at IBM Research – Zurich since 2011. He graduated in Materials Science at the University of Milano-Bicocca, Milan, Italy, in 2003, and obtained his Ph.D in Nanostructures and Nanotechnology in 2006, also in Milan. At IBM, he work atomistic simulations on different type of materials, for example on phase-change materials for storage applications, solid-state electrolytes for batteries. In the last 4 years, he is focused on accelerating the discovery of new materials via a combined use of data analytics and atomistic simulations based on neural networks. He is working on natural language processing tools to extract knowledge from text and deep learning based-models for data-mining and name entity recognition. He is exploring neural-network forcefield to model the atomic interactions.

YOUR NOTES:

THOMAS LEHMANN

Technische Universität Dresden, Germany
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Machine Learning with Python

In a hands-on session on machine learning we discuss the application of various methods, starting from Linear Regression to Random Forests and Cluster Analysis. Apart from a theoretical discussion of those concepts, we will start to implement them in Python. Please bring your own laptop and brush up your programming skills.

Biography

Thomas Lehmann is a Theoretical Physicist with a focus on numerical modelling of quantum transport in nanostructures and molecular electronics. He studied Physics at the TU Dresden and obtained his PhD in the group of Prof. Cuniberti in cooperation with the International Max Planck Research School and the International Graduate School iEGSEMP: Korea with research stays at POSTECH (Korea), CEMES-CNRS (France) and UNIST (Korea). Since becoming interested in Machine Learning methods, he has been awarded a Data Science Fellowship at ASI Data Science in London in 2018. He has been working for easyJet to develop a dynamic pricing model for seat allocations by predicting the time-evolution of customer demand. As a PostDoc he is now looking into applications of Machine Learning models for materials science.

YOUR NOTES:

STEFANIE REESE

RWTH Aachen University, Germany
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Model reduction and data-driven mechanics-development and applications

Data analysis and data science have become fundamental domains in the past decade. Data science has not only a big impact on financial markets but also in engineering areas. Experimental measurements get increasingly reliable and data-rich. To find a description of the usually strongly non-linear material behaviour, complex constitutive laws have to be developed and fitted to the experimental measurements. An interesting alternative idea is the use of the data directly. In our work we intend to use data from experiments to extract pairs of stress and strain to execute computations by evaluating them without constitutive model. Hereby, we bypass any kind of modelling error as well as any problem concerning parameter fitting.

An additional question is the application of data in the context of model order reduction (MOR). We focus here on projection-based MOR and show some ideas to include the data directly.

Biography

Stefanie Reese is Full Professor at RWTH Aachen University and Director of the Institute of Applied Mechanics (IFAM) in Aachen, Germany, which she established in 2010. After receiving her Dr.-Ing. degree in 1994 from the Technische Universität Darmstadt and postdoc stays at the University of California at Berkeley (USA) and the University of Capetown (South Africa) she became in the year 2000 Professor at the Ruhr University Bochum. From 2005 until 2009 she was Full Professor (W3) at the Technische Universität Carolo-Wilhelmina at Braunschweig. She has received several prizes and is member of three academies, among these the National Academy of Science and Engineering. Since 2010, she is Fellow of the International Association for Computational Mechanics (IACM). She is Associate Editor of the open access journal Advanced Modeling and Simulation of Engineering Sciences and holds membership in three editorial boards, e.g. in Computer Methods in Applied Mechanics and Engineering. In 2015, she became Treasurer of the European Mechanics Society (Euromech).

YOUR NOTES:

PATRICK RINKE

School of Science, Aalto University, Helsinki, Finland

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Machine Learning in Materials Science

For many material science problems, quantum mechanical insight is required. Such insight can now be gained by atomistic materials simulations such as density-functional theory (DFT). However, accurate calculations are costly and limited in the tractable systems size (i.e. number of atoms in the calculation) and the number of tractable materials. Machine learning methods can help to overcome this size-accuracy conundrum.

In this lecture, I will take an atomistic view to machine learning in materials science. I will first introduce the basic workflow that governs all machine learning approaches in materials science. Then I will discuss how materials are presented to the machine for optimal learning. Such materials descriptors require insight into the specific materials science question at hand and can have a large influence on the learning success. As machine learning methods, I will present the kernel ridge regression (KRR) approach and artificial neural networks (NNs). I will demonstrate their success and discuss their pros and cons for two examples: molecular excitation spectra and halide perovskite (ABX_3) alloys. I will also briefly discuss data diversity as a factor that influences learning success. Once trained, these machine learning models can make predictions for new systems instantly and at no further cost for the end user. I will illustrate how these models can then be used to gain further materials science insight.

Biography

Prof. Patrick Rinke received his PhD from the University of York in England in 2003. Subsequently, he was a post-doctoral scholar at the Fritz Haber Institute (FHI) of the Max Planck Society in Berlin, Germany, and in the Materials Department at the University of California Santa Barbara (UCSB) before becoming a group leader at the FHI in 2009. Since 2014, he leads the Computational Electronic Structure Theory (CEST) group in the Department of Applied Physics at Aalto University in Helsinki, Finland. He develops advanced electronic structure and machine learning methods and applies them to pertinent problems in materials science.

YOUR NOTES:

FRANK AND HOLGER GROßMANN

Anton Paar GmbH, Germany
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Materials 4.0 can only exist with blockchain solutions

Blockchain technologies have a great potential to map supply and process chains transparently and accurately. The lecture will give an insight into the blockchain technologies and current application examples, which can be seen in direct or indirect relation to materials. In addition, questions are formulated and answered:

- on why the technology can be used in relation to materials 4.0 and Big Data.
- an outlook on future research needs.

Biographies

Frank Großmann

2004 – 2007	Apprenticeship at Deutsche Telekom
2007 – 2010	Network and system administrator
2010 – 2015	Study of business IT (M.Sc.)
since 2016	SAP developer

Holger Großmann

2006-2012	undergraduate and graduate studies BTU Cottbus
2010	Alstom Power Schweiz / Surface Solutions
2011 -2012	Fraunhofer IWS Dresden (diploma thesis *Schmelzmetallurgische Herstellung CNT Verstärkte Aluminiumlegierung*)
2012 – 2016	research associate TU Dresden, Professur für Wasserstoff- und Kernenergietechnik
2017	Dr.-Ing. at TU Dresden (topic *Ablagerungs- und Resuspensionsvorgänge graphitischer Partikel in Heißgasströmungen)*
since 01/2017	Anton Paar Germany GmbH product specialist mechanical surface characterization

YOUR NOTES:

EMRE TOPAL

Fraunhofer Institute for Ceramic Technologies and Systems, Dresden, Germany
Technische Universität Dresden, Germany
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Neuronal networks for the improved reconstruction of X-ray CT data

Neural networks, developed in the 1950s not long after the emergence of Artificial Intelligence research, attempted to simulate the way the brain works though in a greatly simplified form. With the improvements in numerical algorithms and the availability of increasingly powerful computers more and more layers of virtual neurons can be modelled. This progress enables deep learning, and especially neural networks, to beat other machine-learning techniques in image processing and pattern recognition. In the purest form, a neural network is a program that maps out a set of virtual neurons and that assigns random numerical values, or "weights", to connections between them. These weights determine how each simulated neuron responds - with a mathematical output between 0 and 1 - to a digitized feature. If the network does not accurately recognize a particular pattern, a numerical algorithm will adjust the weights. This is the way artificial neural networks can train themselves to recognize complex patterns. In the era of big data, inevitable, deep learning applications have been extended to the field of microscopy and tomography to provide solutions to major issues like artefact reduction and missing data, and furthermore to autotomize the feature detection and segmentation tasks.

The aim of this talk is to introduce some modern machine learning approaches, in particular for applications of deep convolutional neural networks (CNN) to high-resolution X-ray computed tomography, transmission electron microscopy and cryo-electron microscopy data for artefact reduction, noise reduction and pattern recognition. I will also present a novel region-based-CNN with support vector machine classifier for motion compensation, and a CNN for data recovery in high-resolution X-ray computed tomography.

Biography

Emre Topal is a PhD student at the faculty of Electrical and Computer Engineering of Technische Universität Dresden since 2017. His studies include 3D materials characterization and 3D data processing. He received M.Sc. degree in Material Science and Engineering from Bursa Technical University in 2016. From 2015 to 2016, he worked as production engineer at Rexroth-Bosch in Bursa, Turkey. Since 2017 He continues his studies at Dresden Center for Nanoanalysis and Fraunhofer IKTS in Dresden, Germany.

YOUR NOTES:

DANIEL URBAN

Fraunhofer IWM, Freiburg, Germany
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Building a materials database for the digital representation and modelling of materials along the product life cycle

The mechanical properties of materials are largely determined by their microstructure and thereby depend on their history which involves all the steps of processing and machining. The traditional and prospective challenge of material science is to derive process-structure-property relationships which allow the reliable prediction of the mechanical behavior, the limits in the operating conditions and the lifetime of a device. The measurement of mechanical properties has to be systematically embedded into the knowledge about the history of the material specimen. Due to the vast variety of possible processing methods, mechanical properties, characterization methods, analysis tools, and available multiscale models, the material data is usually heterogeneous and in general incomplete. The goal is to represent the material and its history within an ontology based network-graph which can be used for data analysis and further machine learning. Within the project MaterialDigital, funded by the Land Baden-Württemberg, this type of data space is currently build-up at the Fraunhofer IWM for two model applications, namely metals and polymers. This talk will discuss the requirements and the technical structure of the data base as well as the necessary steps for the digital workflow (development of the underlying ontology, structuring of the data, generation of queries). The general procedure and the difficulties along the way will be exemplified by several examples from current research work.

Biography

Dr. Daniel Urban studied physics in Freiburg and Paris and got his diploma in 2002. Subsequently, he did his PhD on the topic of Stability, Symmetry Breaking and Scaling Properties of Metallic Nanowires and in the field of theoretical mesoscopic solid state physics. In 2006 and after two research stays at the University of Arizona, he received his PhD from the University of Freiburg, where he continued to work as a post-doc. His research touched several aspects of charge and spin transport in nanostructures of one, two or three dimensions and made him move to the Universidad Autonoma de Madrid for some time. In 2012, he joined the group Materials Modeling at the Fraunhofer Institute for Mechanics of Materials in Freiburg which he is now heading since 2017.

For his current research he use methods based on quantum mechanics or classical atomistic mechanics and on multi-scale materials modeling in order to develop material models and predict physical, chemical, and mechanical material properties.

YOUR NOTES:

WEIHUI XIE

Shanghai Jiao Tong University, Shanghai, China
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SJTU and Zhi - Hong summer school series

Shanghai Jiao Tong University (SJTU) is one of the higher education institutions which enjoy a long history and a world-renowned reputation in China. Shanghai Jiao Tong University (SJTU) pioneered in setting up the discipline of Materials Science and Engineering in China, and the first major of heat treatment was set up in 1952. The discipline of 'materials science and engineering' has been consistently ranked top 0.1% in ESI.

The "Zhi-Hong" International Summer School of Advanced Materials (ISS-AM) is organized by School of Materials Science and Engineering (SMSE) at SJTU, aiming at promoting the interactive cultural and academic exchange between top-level scholars and students from all over the world. "Zhi-Hong" ISS-AM is a two-week program with one theme every year. The themes are "Advanced Metallic Materials", "Advanced Functional Materials" and "Advanced Materials Processing" respectively. The "Zhi-Hong" ISS-AM offers lectures and professional practice to the students, e.g. student seminars, visits to research laboratories, culture festival, field trips and culture tours in Shanghai.

After 4 years of development, the "Zhi-Hong" ISS-AM has become one of the best summer school programs in SJTU and attracts more and more international and Chinese students.

Biography

Ms.Weihui XIE is a coordinator for international education affairs at School of Materials Science and Engineering (SMSE) in Shanghai Jiao Tong University (SJTU). She received her B.E. in Polymer Science and Engineering in 2006, and her M.S. in Chemistry in 2008, both from Zhejiang University. She has been engaged in administration of graduate education and international education for 7 years. As one of the key organizers, she has organized 4 sessions of SJTU "Zhi-Hong" International Summer School of Advanced Materials which has become one of the best summer school programs in SJTU.

YOUR NOTES:

BENJAMIN KLUSEMANN

Leuphana Universität Lüneburg, Germany
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Application of machine learning approaches in the context of processes and materials with focus on artificial neural networks

Machine learning tools offer exceptional opportunities for material scientists and engineers to achieve a throughout identification and quantification of essential features along the process-structure-property-performance chain that might otherwise not be obtained or accessible. This substantial gain in knowledge can help in the development and improvement of materials, processes and techniques. In this regard, it is essential to understand, capabilities and limitations of different machine learning and other data mining approaches to select the correct method for a specific application. Therefore, this lecture will provide a discussion on a selection of successful applications in the literature of machine learning approaches to specific problems in the field of continuum materials mechanics [1]. We categorize them as descriptive, predictive or prescriptive according to their designated type of task. Different examples will be reviewed, involving the application of different types of artificial neural networks, support vector machines or model order reduction procedures such as principal component analysis, among others. These techniques can be applied, to accelerate the identification of material parameters, to support design and optimization of novel processing routes or materials, or to better understand and predict fatigue behavior, among other aims. There will be an in-depth discussion on two examples of successful application of artificial neural networks to identify key dependencies within a material as well as to improve and correct complex measurement devices. Selected examples of different machine learning methods will be illustrated in a hands-on-session.

Biography

Benjamin Klusemann studied mechanical engineering at the TU Dortmund. Subsequently, he did his PhD in computational mechanics at TU Dortmund as well, graduating in 2010 followed by a postdoctoral period at the RWTH Aachen. In 2012, he moved to the TU Hamburg to join the institute of continuum mechanics and material mechanics as senior researcher. With a Humboldt fellowship, he joint Caltech, USA as postdoctoral scholar in 2013. Since 2015, he is professor for local engineering, in particular process simulation at the Leuphana University of Lüneburg. Between 2015 and 2019 he was head of the working group "Residual stress engineering" and since 2019 he is head of the department "Solid State Joining Processes" at the Helmholtz-Zentrum Geesthacht. He received a number of awards, including the Richard-von-Mises-Prize of GAMM 2017 and the ESAFORM scientific prize 2019. His research interests include various aspects of computational mechanics, including aspects of micromechanics, multi-scale modeling or data-driven modeling. Furthermore, he is particular interested in technological processes such as solid-state joining, local modification as well as additive manufacturing techniques, both from experimental as well as numerical point of view.

YOUR NOTES:

REBECCA JANISCH

ICAMS, Ruhr-Universität Bochum, Germany
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Atomistic aspects of deformation and fracture

In this lecture we will have a look at the mechanical properties of metals and alloys, such as stiffness, strength, and fracture toughness, as selection criteria for materials design. After looking at some macroscopic manifestations of these properties, we will have a look at the microscopic processes behind these terms - lattice distortions, dislocation motion and crack propagation - and then focus on the atomistic (and partially electronic) origins of these processes. Finally, different methods to simulate mechanical deformation on the atomic scale and to extract mechanical properties of micro- and macro-structures will be introduced.

Biography

Rebecca Janisch studied Physics at the University of Stuttgart, from where she received her PhD in 2003. During the research for the PhD thesis at the late Max-Planck Institute for Metals research in Stuttgart she became familiar with the atomistic aspects of interface properties. Related phenomena followed her around during several postdoctoral research stays in Santa Barbara, Chemnitz, and Erlangen. Since 2008 she is leading the group “Mechanical Properties of Interfaces” at the Interdisciplinary Centre for Advanced Materials Simulations (ICAMS) at Ruhr-University Bochum, where she was habilitated in 2017.

YOUR NOTES:

MARC–ANDRÉ KEIP

Universität Stuttgart, Germany
* E-Mail: marc-andre.keip@mechbau.uni-stuttgart.de

On the use of machine learning methods in multiscale modeling

In recent years, there has been an ever increasing impact of machine learning on science, engineering, economy and also our private lives – may it be the detection of tumors on X-ray images, autonomous driving of automobiles or recommender systems for web applications. The combination of vast amounts of available data and growing computational power has enabled machine-learning methods at large scales. The integration of related methods in classical engineering fields such as material modeling and computational mechanics seems thus promising. This applies particularly to multiscale scenarios, where associated methods could find use not only in surrogate-model development or image recognition, but also in the numerical discretization of the problem itself.

The present lecture provides a short overview on potential applications of machine learning in computational mechanics. Focus is on material modeling and the numerical discretization of multiscale problems by artificial neural networks. In a hands-on-session, students will learn to use TensorFlow® to set up exemplary machine-learning codes themselves.

Biography

Marc-André Keip studied Civil Engineering at the University of Duisburg-Essen (UDE) and graduated as Diplom-Ingenieur in 2004. After two and a half years in industry, he returned to UDE to pursue doctoral studies in applied mechanics. In 2011, he graduated as Doktor-Ingenieur with a dissertation on multiscale modeling of electro-mechanically coupled boundary value problems. After two further years at UDE and a research stay at the California Institute of Technology, he became Junior-Professor at the Cluster of Excellence in Simulation Technology at the University of Stuttgart in October 2013. From 2016 through 2019, he lead the Chair of Materials Theory at the University of Stuttgart as substitute Professor. In November 2018, he was awarded the "Lehrepreis der Universität Stuttgart" for special achievements in teaching. Since January 2019, Marc-André Keip is Professor of Applied Mechanics (Materials Theory) at the Department of Civil and Environmental Engineering at the University of Stuttgart. His research interests are in the area of continuum mechanics, material modeling and simulation methods. Particular interests include multiscale and multifield problems, phase-field modeling as well as data-driven simulations.

YOUR NOTES:

FELIX GÖKÜZÜM

Universität Stuttgart, Germany
* E-Mail: felix.goekuezuem@mechbau.uni-stuttgart.de

On the use of machine learning methods in multiscale modeling: hands-on session

In recent years, there has been an ever increasing impact of machine learning on science, engineering, economy and also our private lives – may it be the detection of tumors on X-ray images, autonomous driving of automobiles or recommender systems for web applications. The combination of vast amounts of available data and growing computational power has enabled machine-learning methods at large scales. The integration of related methods in classical engineering fields such as material modeling and computational mechanics seems thus promising. This applies particularly to multiscale scenarios, where associated methods could find use not only in surrogate-model development or image recognition, but also in the numerical discretization of the problem itself.

The present lecture provides a short overview on potential applications of machine learning in computational mechanics. Focus is on material modeling and the numerical discretization of multiscale problems by artificial neural networks. In a hands-on-session, students will learn to use TensorFlow® to set up exemplary machine-learning codes themselves.

Biography

10/2013:	Bachelor of Science in Environmental Engineering at the University of Stuttgart
08/2014 – 12/2014:	Studies at the Tampere University of Technology (TUT) in Finland
10/2015 – 12/2015:	Research Stay at the California Institute of Technology with Prof. Dennis Kochmann
03/2016:	Master of Science in Environmental Engineering at the University of Stuttgart
10/2010 – 03/2016:	Scholarship of the Studienstiftung des deutschen Volkes
04/2016 – now:	Ph. D. candidate at the Institute of Applied Mechanics at the University of Stuttgart

YOUR NOTES:

ANJA WASKE

Bundesanstalt für Materialforschung und -prüfung (BAM) and
Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden
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Non-destructive testing of materials and composites

Functional materials for energy conversion are important technology drivers needed for the implementation of low carbon energy. Therefore, researchers commonly focus on improving the intrinsic properties of a functional material. However, for applications, the extrinsic properties are at least as important as the intrinsic ones. Consequently, it is important to investigate and understand the external and internal structure of semi-finished products and especially defect dependent properties. The extrinsic properties may change during application and the life cycle of the material as well as through processing and molding steps. Our studies show how X-ray tomographic (XCT) investigations can contribute to structure investigations in composites and massive samples using the example of magnetic materials for energy conversion. The components are tested non-destructively in 3D in order to localize and characterize cracks, pores, inclusions as well as other defects and their influence on the functional properties and also “in-time” during the life cycle of the material. Ex-situ and in-situ experiments performed with non-destructive XCT are predestinated to follow damaging mechanisms of materials under certain load conditions, atmospheres or liquids, e.g. went through several working cycles of a functional material. By combining microtomography with other methods of magnetic and classical material characterization, unique statements about the structure and the functional properties can be made.
From the applications point of view, sometimes complex, three-dimensional geometries are needed to fully exploit the functional properties of the materials, e.g. to ensure a high surface area for heat exchange. Since many functional materials are brittle and difficult to form, shaping is often a big challenge. In principle, additive manufacturing processes offer the possibility to produce complex, porous components from poorly formable alloys. If all stages of additive manufacturing are accompanied by X-ray tomographic imaging, the process of finding the optimal parameters for material processing can be significantly accelerated. Based on the quality control of the initial powder material used and also investigations of the shape and arrangement of defects within the molten structure and their relationship with the melting path scanning strategy, X-ray tomography has proven to be an ideal tool for additive manufacturing, even for functional materials. Overall, tomographic methods are important tools for the development of functional materials to application maturity.

Biography

Anja Waske is the head of division “Radiological Methods” at the Federal Institute for Materials Research and Testing (BAM) based in Berlin, Germany. She studied physics at the Technische Universität Dresden, Germany, followed by a PhD degree in the field of x-ray tomographic characterization of granular matter. Her research interests include magnetic composites and magnetocaloric materials for cooling and energy-harvesting applications. She develops three-dimensional image-analysis methods for understanding the properties of functional and additively manufactured materials.

YOUR NOTES:

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From margins to mainstream: the emergence of data-driven materials research as a field of science and business

From margins to mainstream: the emergence of data-driven materials research as a field of science and business

Data-driven materials science is heralded as a new paradigm in materials research that offers unprecedented opportunities for the discovery of new or improved materials or materials phenomena. Relying on a qualitative, ethnographic study of the emerging field of data-driven materials science, we explore the emergence of this new paradigm as a field of science and business. We base our study on a combination of archival data, interview data and ethnographic field notes collected in key scientific dry-labs and at foundational events and conferences worldwide. We will present the historical development and current status of this field, from the early adoption of open science to the rapid expansion of materials data discovery platforms under the current AI-hype. We will explore the multiple factors that fueled its development and discuss the various (social) challenges that underlie the future development of this field.

Biography

Dr. Amber Geurts is Researcher Technology & Innovation at TNO, Netherlands Organisation for Applied Scientific Research. She is also a visiting research fellow at Aalto University, School of Business and School of Science. Her research focuses on how new technologies and industries emerge and develop. In her studies, she explores these topics from multiple theoretical perspectives. Empirically, her research draws on extensive qualitative and quantitative datasets on, for example, the development of the digital music industry or data-driven materials science. Her research has been awarded several grants, and has been published in various outlets including Advanced Science, Technological Forecasting and Social Change, Journal of Cross-Cultural Psychology, and the Journal of Economic Issues. Amber completed her PhD in Innovation Management at the School of Economics & Business of the University of Groningen in the Netherlands. Her PhD research has won the 2018 ISPIM Innovation Management Best Dissertation Award.

YOUR NOTES:

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Materials Innovation Driven by Data and Knowledge Systems

Emerging concepts and toolsets in Data science and Cyberinfrastructure can be strong enablers for systematic mining and automated capture of Materials Knowledge and its dissemination to distributed cross-disciplinary teams engaged in materials innovation efforts. A data-driven framework is also foundational to the development and implementation of autonomous explorations of the unimaginably large materials and process design spaces while synergistically leveraging all available experimental and simulation data. Although tremendous progress has been made in the development and validation of a wide range of simulation toolsets capturing the multiscale phenomena controlling the material properties (e.g., fatigue performance of advanced materials) and performance characteristics of interest to advanced technologies, their systematic insertion into the materials innovation efforts has encountered several hurdles. The ongoing efforts in my research group are aimed at accelerating materials innovation through the development of (i) a new mathematical framework that allows a systematic and consistent parametrization of the extremely large spaces in the representations of the material hierarchical structure (spanning multiple length/structure scales) and governing physics across a broad range of materials classes and phenomena, (ii) a new formalism that evaluates all available next steps in a given materials innovation effort (i.e., various multiscale experiments and simulations) and rank-orders them based on their likelihood to produce the desired knowledge (expressed as PSP linkages), and (iii) novel higher-throughput experimental assays that are specifically designed to produce the critically needed fundamental materials data for calibrating the numerous parameters typically present in multiscale materials models. I will present and discuss ongoing research activities in my group.

Biography

Surya Kalidindi is a Regents Professor, and Rae S. and Frank H. Neely Chair Professor in the Woodruff School of Mechanical Engineering at Georgia Institute of Technology, Georgia, USA with joint appointments in the School of Materials Science and Engineering as well as the School of Computational Science and Engineering. Surya earned a Ph.D. in Mechanical Engineering from Massachusetts Institute of Technology in 1992, and joined the Department of Materials Science and Engineering at Drexel University as an Assistant Professor. After twenty years at Drexel University, Surya moved into his current position at Georgia Tech. Surya's research efforts have made seminal contributions to the fields of crystal plasticity, microstructure design, and materials informatics. Surya has been elected a Fellow of ASM International, TMS, and ASME. In 2016, he and his group members have been awarded the top prize as well as one of the runner-up prizes in the national Materials Science and Engineering Data Challenge sponsored by the Air Force Research Lab in partnership with the National Institute of Standards and Technology and the U.S. National Science Foundation. He has also been awarded the Alexander von Humboldt Research Award, the Vannever Bush Faculty Fellow, the Government of India's Vajra Faculty Award, and the Khan International Award.

YOUR NOTES:

CONTRIBUTED TALKS AND POSTERS

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Controlled Manipulation of Individual Molecules on Surfaces and Comparison with Machine Learning Approaches

With the continued development of scanning probe microscopy techniques, manipulation of single molecules has become possible. Thereby, the manipulation path can be chosen at will and energy barriers between potential minima on that pathway can be quantified, as can the energy landspace around the molecule before and after manipulation. To explore the practicality of this novel pathway to catalysis research, we selected benzene molecules on a Cu (100) surface as a model system. As Fig. 1 summarizes, we first choose a specific manipulation path and then move the tip at constant but continuously reduced heights z along this path (x coordinate) while recording the oscillation amplitude A and phase phi with the microscope operated in our recently developed tuned-oscillator (TO) detection scheme [1]. To preserve the accurancy of recovered tipsample interaction potentials and forces, we use oscillation amplitudes significantly larger than the decay length of the tip-sample interaction potential [2,3]. Analyzing the full (x, z, A, phi) data array then allows recovery of the potential energy U(x, z) acting between the tip and the sample (Fig. 1b), the force on the tip normal to the surface vertical tip-sample force Fn(x, z) (Fig. 1c), and the force Fl(x, z) that acts on the tip along the manipulation path (i.e., lateral; Fig. 1d) with meV, pN, and pm resolution. In 54 distinct maniupluation events, the molecules were either pushed, pulled, jumped to the tip, or did not move depending on the chemical surronding of the molecule and the chemical identity of the tip. For further insight, we compared the experimentally measured energy landscapes and manipulation outcomes with computational results obtained using a Bayesian Optimization Structure Search (BOSS) protocol. This machine learning technique developed at Aalto University delivers the minimum energy pathways and entire energy landscapes with minimal computational effort.

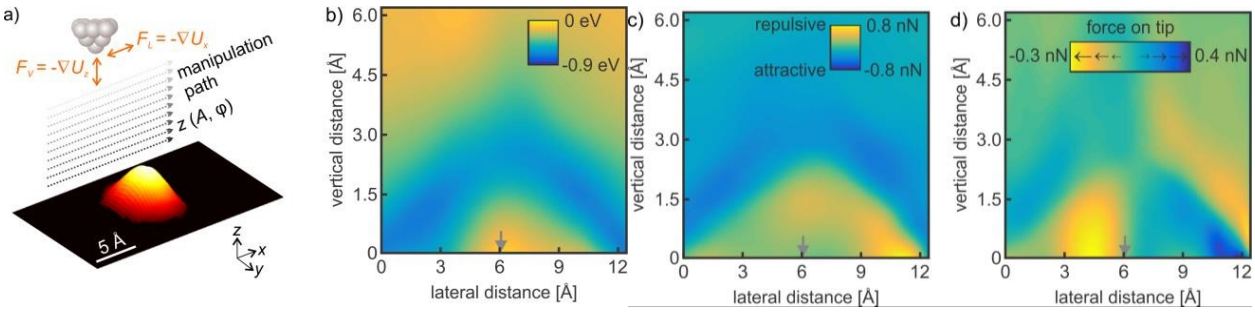

Fig 1: (a) Illustration of the measurement principle; the pseudo-3D image was recorded using STM and shows the benzene molecule studied in panels b-d. (b-d) x-z plots of the potential energy (b) and the forces acting on the tip normally (c) and laterally along the direction of the path (d).

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YOUR NOTES:

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Data Mining of Dislocation Microstructures: Approximating Dislocation Curvature

An immense amount of discrete dislocation dynamics and experiment method data are generated everyday but none of them having a straightforward information concerning the dislocation curvature. Apparently, the approximation of the curvature depends on the qualitative approach. Starting from the stated problem, the need of quantitative approach is necessary since the curvature is the one of parameters determining the physical properties such as local line tension, stress field, etc. Thus, the development of a surrogate model for determining the dislocation curvature is done within this work utilizing data mining framework. The output of learning is a surrogate model for predicting the so-called smoothing factor as a target property. The involvement of estimators, e.g., ordinary least square (OLS), least absolute shrinkage and selection operator (LASSO), and ridge regression method, coupled to principal component analysis (PCA), could be used further to analyze the feature importance building a model and identify the model outliers.

YOUR NOTES:

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Plasmonic Nanocatalysis - Do shape and size matter?

Plasmonic nanoparticles (PNPs) are widely used in many different technological applications ranging from nanomedicine to biosensing. Recently, Au PNPs have been proposed as a source of energetic electrons excited via surface plasmons, and exhibit efficient photocatalytic properties in the field of solar energy, energy harvesting and conversion by splitting of water and hydrogen molecules, and thus hydrogen production for clean energy generation. Since gold, silver and aluminium exhibit the resonance in the UV and visible regime, they are of particular interest for solar energy conversion. In this research, we shall principally be interested in the role played by local geometry, chemical ordering and the number of Au and Au-Pt atoms.

Understanding the performance of plasmonic nanostructures for water splitting will require an atomistic investigation of geometrical and electronic structure versus PNP size and chemical composition using both standard and time-dependent density functional method (DFT and TD-DFT). Indeed it has been recently observed that the geometry might play a fundamental role in determining the features of the spectrum (e.g. the frequency of the localised surface plasmon). The initial modelling results will provide a roadmap for planning experiments, and, in turn, specific experimental configurations will be modelled to provide an understanding of experimental results.

YOUR NOTES:

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Understanding alloy compositions and strain-hardening of TWIP Ti alloys: Material informatics and dislocation-based modelling

Titanium alloys have been serving as structural materials for aerospace applications, owing to their high specific strength (strength-to-weight ratio), corrosion resistance and attractive fracture toughness (the energy required to for propagating cracks). The unique {332}<113> mechanical twinning system provides TWIP (twinning-induced plasticity) Ti alloys a huge play ground to push forward the boundary of strength and plasticity. Material informatics in terms of alloy compositions and mechanics data are collected and rebuilt via electronic structure calculations, which provide an efficient guideline for alloys design. A new quaternary Ti-11Mo-5Sn-5Nb (wt.%) alloy was developed, exhibiting significant uniform elongation through good strain-hardening owing to the formation of a high volume fraction mechanical twins. A multiscale constitutive model was built to prescribe the microstructure evolution and strain-hardening of {332}<113> TWIP Ti alloys. This model not only incorporates the effect of enhanced dislocation storage term by reduced dislocation mean free path, but also highlights the contributions of kinematic hardening due to the internal stress field concentrated at coherent twin/β-matrix interfaces. The present model was verified to the new Ti-11Mo-5Sn-5Nb alloy as well as a series of Ti alloys undergoing {332}<113> twinning at different deformation conditions. The evolutions of twinning volume fraction, intertwin spacing, dislocation density and strain-hardening were successfully described. Particular attentions were placed on strain-rate-sensitivity of twinning kinetics, critical strain for twin nucleation and dislocation annihilation.

YOUR NOTES:

POSTERS

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Quantification of sheet nacre morphogenesis using X-ray nanotomography and deep learning

High-resolution three-dimensional visualization is key to our understanding of biological tissue formation and function. Recent developments in synchrotron-based X-Ray tomography techniques are capable to provide unprecedented morphological information on relatively large sample volumes with a spatial resolution of down to 10 nm. However, the analysis of the data and its segmentation still presents a significant challenge, especially when considering complex biomineralized structures that exhibit hierarchical arrangement of their constituents across many length scales – from millimeters down to nanometers. In the present work, synchrotron-based nanotomography combined with state-of-the-art machine learning image processing methods are successfully employed to image and investigate the nacreous architecture in the bivalve *Unio pictorum* in 3D. Furthermore, using kinetic and thermodynamic considerations borrowed from physics of materials, the obtained spatial information is used to provide an analytical description of structural and topological evolution of nacre during shell formation. Hence, this study not only establishes a workflow for high-resolution three-dimensional analysis of fine highly-mineralized biological tissues, but also provides a detailed quantitative view on nacre morphogenesis.

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Rigid-body docking and molecular mechanics: a novel approach to the rational design of nano/bio composite materials

Novel material discovery still relies heavily on a trial-and-error approach. Investigation of novel materials requires experimental synthesis and accurate characterization, which are common bottlenecks. The combination of the two factors severely hampers research in the field of innovative materials.

By combining methods commonly employed in Computer Aided Drug Design, we developed a protocol for the efficient design of protein - Carbon Nano Particles (CNPs) hybrids for nanomedicine applications. Assemblies of proteins and CNPs show great promise for nanotechnology, materials science and medical applications [1]. In particular, gadofullerenes are a novel alternative to commercial Magnetic Resonance contrast agents as they yield a higher signal at significantly lower concentrations [2]. Their medical applications are limited by their tendency to form aggregates in physiological conditions. Protein-CNPs are water soluble and disperse monomolecularly [3]. To identify a suitable carrier protein for Gd@C82, we performed docking-based inverse virtual screening on the 1103 protein structures of a large structural database using rigid-body docking programs. The propensity for formation of protein-Gd@C82 assemblies was coarsely ranked using the scoring functions of the docking programs. The most promising hybrids underwent a stepwise Molecular Mechanics minimization protocol in which the least stable structures were discarded. The binding energy of the most stable hybrids was computed accurately using the MM/GBSA method. This protocol led to the identification of potential carrier proteins, such as cytochrome P450, and pharmacological targets, which will be experimentally tested in the future.

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Computational study of solvent effect on aggregation of core-chlorinated naphthalene tetracarbonxylic diimide and its interaction with solvent molecules

The project I am currently working on is to study the solvent effects on the crystal habit of an organic semiconductor material, naphthalenetetracarboxylic diimides (NTCDI). Not surprisingly, some dihedral parameters of this recently developed material are missing in the commonly used OPLS force field. Moreover, these dihedrals overlapped at adjacent positions which made the parametrization even harder. After accessing my method against those in previous studies, and testing different optimization techniques, I successfully obtained good fitted parameters. Later, I realized that the OPLS force field might underestimate, or otherwise poorly represent, the important π-π interactions in aromatic molecules. This was the case in my system so that I evaluated the accuracy of these parameters in the force field and tailored it for my project.

I was able to complete the molecular dynamics simulations in different solvent systems to calculate the binding energy of two NTCDI molecules. I also found that the NTCDI molecule exhibited two (yet experimentally unseen) local energy-minimum conformations. I investigated the energy barrier controlling the interchange of these two conformations using the Nudged Elastic Band method and a continuum solvation model based on the solvent electron density. To answer the question of how individual NTCDI molecules evolved in molecular dynamics, I sampled the frequency at which each conformation was present in a given solvent system. Moreover, to further investigate the behaviors of NTCDI in solvents from a thermodynamic standpoint, I used steered molecular dynamics to sample an unbiased pathway that two NTCDI molecules will take when you slowly pull them apart. Then I used thermodynamic integration to get a more accurate ensemble average along the pathway to calculate the potential mean force. These results were consistent with experimental findings and offered additional insights of the thermodynamics properties of NTCDI in solvents.

To extend the scope of my project, I am working on the charge transport properties of NTCDI crystal. I am calculating electron transfer integral calculation of NTCDI dimers using Marcus theory and recently developed constrained DFT for excited state calculation. I will also investigate the electronic properties of the unit cell with ab initio molecular dynamics.

Besides my thesis work, I have experience on general coding and machine learning related projects. Along the research work, I have developed Python scripts to process large dataset. My goal is to write robust code and to efficiently analyze the time-series data with minimum human supervision. I have also worked on a machine learning project about breast cancer diagnosis. I built models based on the breast cancer diagnosis and cancer cell features and compare the accuracy of different machine learning models. The models I used are decision tree, principal component analysis and linear regression. For example, I used principal component analysis to classify the cancer diagnosis and make predictions based on T^2 and SPE statistics. I used benign diagnosis as training model and scaled its covariance matrix. I chose the cumulative variance ratio as 90%, which resulted six principal components to be used. Then I compared the T^2 and SPE statistics of malignant data to validate the success rate of my model.

DCMS MATERIALS 4.0 SUMMER SCHOOL

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Data-Driven Simulation in Continuum Mechanics

Numerical simulation in classical mechanical engineering is based on the usage of two different classes of equation. The first class is related to conservation laws and derives from universal principles. These laws are applied to derive differential equations to describe the behavior of the object to be considered. Whereas the second class of equation is based on constitutive relations formulated through experimental observation e.g. material laws. As a result most of the existing material models lack of generality and need to be constantly adapted to describe new experimental finding. Considering the imperfect knowledge of the functional form of material laws and scatter and noise in the experimental data, this modeling process adds error and uncertainty to the solution. Thus the class of equations based on conversation laws is mired in empiricism and arbitrariness. To resolve the issues with empirical material models, T. Kirchdoerfer and M. Ortiz introduced a new computing method for linear elasticity problems, called data-driven computing. The paradigm bypass the material modeling by using all material data directly to perform numerical simulations. Consequently, empiricism, error and uncertainty in the process of material modeling are eliminated.

One aim of the study is the research and improvement of data-driven solvers related to deep neural networks. One approach is the expansion to more complex problems for example problems with inelastic material behavior will be taken into consideration. Since inelastic materials raise the fundamental problem of sampling history-dependent material-behavior, the use of Data Science and Big Data tools must be expected. In connection with data-driven solvers, the entire numerical simulation could be reformulated and solved by a deep neural network. Accordingly the task is to investigate the possibilities of machine learning and data-driven computing to improve the process of material modeling.

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Experimental and simulation study to create efficient welding on silver nanowire networks

The rapidly growing interests in recent years for flexible and transparent optoelectronics devices have imposed a major challenge to develop materials combining mechanical flexibility with high electrical conductivity and optical transmittance. On transparent and conductive applications, Indium Tin Oxide (ITO) is one of the most commonly used materials due to its great combination of electrical and optical properties. Nonetheless, 1D metal nanowire networks and specifically silver nanowires (AgNW) are arising to replace ITO showing comparable or even better electrical and optical properties together with improved mechanical flexibility (ITO is a brittle material). AgNW networks also bring potential lower costs, as the material use per unit area is considerably decreased [1]. Although AgNW have such outstanding features, there are some issues associated with stability due to their low adhesion to the substrate with associated surface roughness and the need to avoid high temperatures (>200 ºC) due to heat-sensibility [2].

Moreover, the electrical conductivity of AgNW networks can still be improved. AgNW are surrounded by a layer of Poly(vinylpyrrolidone) (PVP) surfactant to improve the stability of the nanostructures in powder form/solution, resulting in non-ideal NW-to-NW electrical contact. Thermal annealing at temperatures near to the melting of PVP (~200 ºC) can increase the electrical conductivity of AgNW networks by opening free paths for surface diffusion of silver atoms, leading to the formation of joints between two contacting wires [3]. Mechanical pressure acts on a second step to improve the adhesion to the substrate and to increase the contact area/number of contact points between AgNWs in networks.

In this study the aim was to analyse the influence of mechanical pressure and thermal annealing, analysing the conformability of AgNW networks when submitted at high pressures to create welding points. In this study the electrical conductivity was also studied comparing the values before and after applying mechanical pressure. Here the study was divided into two parts: experimental and simulated models.

On experimental study, commercial AgNW (10 µm length, 100 nm diameter) were spray coated at 150 ºC into glass and flexible subtrates (PET). Spray coating is one of the most attractive methods for large area electronics creating a uniform deposition of AgNW networks under a controlled environment [2]. Thermal annealing was tested under several conditions (until 300 ºC) and afterwards AgNW networks were submitted to mechanical pressure for welding the nanowire networks. A remarkable electrical conductivity of 5 Ω/sq could be obtained with these experiments.

To understand these results, a simulation using Finite Element Analysis (FEA) was performed using a commercial software (ANSYS). In this simulation, the experimental results were inserted into the characteristics of AgNW, the length of a nanowire was 10 times its diameter and the boundary conditions of surface effects were neglected. Different meshes with increasing element densities have been used to test the convergence of the solution. Structural models using AgNW were performed to analyse the local strain and deformation

of the material under mechanical pressure. Thermal and electrical models were also studied to compare with the experimental results.

On a material level, there is a huge gap on numerical simulations and specifically on nanostructures there is still a lot of work to do on computational modelling [4]. These preliminary results can open a wide world of new studies and applications on flexible electronics, with huge potential for expansion into other material systems.

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STM visualisation of grain boundaries on the surface of nanocrystalline copper (111) films

Nanocrystalline Copper films were prepared by deposition on 7 nm Tantalum thin layer on Silicon are studied using Scanning Tunneling Microscopy. The films had thickness less than 50 nm and grain surface is (111) orientated. In this study, defect structures including dislocations, low angle grain boundary and high angle grain boundary with [111] tilt axis are identified on the surfaces of annealed samples using Low Temperature STM.

In this work, a global out-of-plane rotation of adjoining grains of low angle grain boundaries is found[1]. For high angle grain boundary, a local out-of-plane rotation along the triple junction is found, in contrast to Mullins' grooving. However, the dynamics of this out-of-plane rotation is still unknown [2].

The underpinning dynamical processes such as single dislocation movement at surface, the dislocation interactions and dislocation recovery are far from being well understood. Films with Burgers vectors of dislocation at the surface plane and [111] tilt grain boundaries is a simple system to start with. Variable Temperature STM provides a possibility to observe these grain boundary dynamics, including grooving and diffusion mechanisms at elevated temperatures and understanding of surface stability and surface reactions, which are critical to the rotation kinetics.

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Relevance of Numerical Drift-Diffusion Simulation for Unravelling the Functioning of Light-Emitting Electrochemical Cells

After more than two decades of research involving experiments and modeling studies, the basic operation principles of light-emitting electrochemical cells (LECs) seem to have been firmly established. Contrary to that claim, we demonstrate here that the analysis of a moving emission zone (EZ) in the active layer of sandwich (400 nm thick) super yellow polymer LECs affords surprises and far reaching insights into the functioning of LECs. Since the interplay of ions and charges is very complex, numerical drift-diffusion modeling was necessary to fully understand the measurement data.

We support this view first with results from low frequency capacitance measurements that are commonly related to the dynamics of the low-conductivity intrinsic part of the p-doped/intrinsic/n-doped junction in the device. The results are contradicting the common believe that the optimal electrical performance is reached when the doped regions are fully established. We explain our observations of a moving EZ and the transient capacitance data with results from electrical simulation and find that the sole pre-condition for these events to occur is that the mobilities of the anions and cations are not equal. From the direction of the emission zone shift, we can further deduce that the mobility of the cation in our case must be larger than the mobility of the anion. Quantitative Tof-SIMS profiles at different times during operation show that the displacement of anions stops at the same time when the capacitance levels off, confirming the relation between ion movement and the observed EZ shift and capacitance dynamics. Our results provide a simple explanation for the often observed EZ shift in LECs, and we show that numerical simulation is a necessity to understand the dynamics in these polymer LECs.

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Influence of oxidation on the mechanical response of Aluminum Foams by using molecular dynamics simulations

Lightweight but remaining high stiffness is one of the most outstanding properties of that make material of metal nanofoams widely used. Because of its high ratio between surface and volume accompanied with affinity of oxygen, this type of material will dramatically be affected by oxidation. In this study, simulation of molecular dynamic will be employed to investigate the effect of oxidation on Aluminum nanofoam. To be more specified, the oxidized Aluminum nanofoam shows higher flexibility without reducing tensile strength.The explanation for this can be the fact that the increase in nucleation defect proportion at interface between Oxygen atoms and Aluminum atoms which is able to prevent deformation. Simultaneously, concentration of Oxygen increases due to decrease of enthalpy. This will strengthen the bond in Al203 nanofoam.

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Interactions of ions across carbon nanotubes

Carbon nanotubes (CNT) are one of the most promising novel forms of carbon. Because of their high storage capacity for ions, they hold great promises for applications in Li-ion rechargeable batteries and supercapacitors [1,2]. The interaction of ions across the walls of CNTs is a key factor in the functioning of such devices. In a previous work [3], we discovered an unexpected effective attraction between two Li ions separated by a semiconducting nanotube. This results explained experimental evidence for an attractive interaction between Li-ions in batteries [4,5]. In the present work, we have systematically studied the inter-ionic interactions by changing the nature of the nanotube (semiconducting or conducting), as well as the type of ions. Thus we placed pairs of Li / Li and Li / Cl ions on opposite sides of the wall of a nanotube and investigated their interactions with density functional theory. Li donates an electron to CNTs without forming a chemical bond. Therefore the adsorption of a first Li-ion increase the electronic density of states at the Fermi level of the CNT making the adsorption of a second ion more favorable. This effect is stronger for semiconducting (8, 0)CNT, but persists for conducting (5, 5) tubes. In contrast, Cl accepts an electron from the CNTs and forms a chemical bond. This induces an increase of the work function, which again favors the adsorption of a Li-ion on the other side of the wall. The direct Coulomb interaction between ions on opposite sides of the wall is small; the attraction or repulsion is caused by the modification of the electronic properties of the intervening CNT.

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Virtual Manufacturing and Prototyping for Improvement in Automotive Crash Performance

Recent lightweight programs and regulations in automotive industry and especially for structural body components are pushing the adoption of innovative steels, such as Advanced High Strength Steels (AHSS) grades, including dual-phase (DP) steels and martensitic boron hot-formed steels, with both high strength and good formability. These stronger grades allow further weight optimization at the sheet metal level but may show some degraded properties around the welds due to unwanted heat-treatment. Indeed welding involves complex interactions between thermal, metallurgical and mechanical phenomena. These interactions generate residual stresses and distortions in a welded structure, affect the heat affected zone (HAZ) properties and can significantly affect the performance of the product. The degraded zone can trigger cracks with a risk of propagation to the whole body in a crash scenario.

We propose computer aided assessment of the complete manufacturing process from stamp to weld and assembly to control dimensional inaccuracies inside the structural BIW components. The mechanical properties of the various metallurgical components are then tested and modelled for use in crash simulation in order to improve failure prediction of weld joints. Meso scale models of spot weld with account of manufacturing have been developed to predict weld rupture and capture local cracks. These models can then be integrated in car crash simulations with a multi-scale modelling approach.

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Piezoelectric Hafnium Oxide Thin Films

This paper presents the piezoelectric properties of silicon doped hafnium oxide (Si:HfO_2) thin films and their superior suitability for energy harvesting applications. Various layer thicknesses from 10 nm to 50 nm, executed as single layer and in a laminate structure, were deposited. The piezoelectric coefficient $d_{33,f}$ of the samples was measured via double beam laser interferometry (DBLI) and converted into d_{33} based on a numerical simulation model which results in values of up to d_{33}=73 pm/V (PZT: 21 pm/V @ 1µm). Additionally, the Curie temperature is investigated for enabling a temperature assisted poling. Finally, the Si:HfO_2 films were electrically investigated by evaluating the relative permittivity between 37 and 56.

Keywords: Piezoelectricity; Hafnium Oxide; Energy Harvesting; Cantilever; Thin Film

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Molecular dynamics study of shock waves in ironcarbon single crystals

Shock compression experiments in pure iron show a three-wave structure: an elastic wave, a plastic wave and the phase-transformation from α- to ε-iron. This three-wave structure has been confirmed by both experiments and molecular dynamics (MD) simulations. Large-scale MD studies provide insights into the transformation kinetics of iron including the transformation mechanisms, stacking faults and twins in ε-iron and the orientation dependence of iron single crystals. However, the influence of carbon on the transformation process remains an open topic. By atomistic simulations of high-strain rate compression of iron-carbon, we show that carbon decreases the elastic limit, but strongly increases the transformation pressure. We examine the role of carbon in the material transformation process under intense shock wave loading in Fe and Fe-C single crystals.

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The Big Bang Theory: Towards Predicting Impact Sensitivity of Energetic Materials

Energetic materials (explosives, propellants and pyrotechnics) are used in a broad range of applications. Some are used for entertainment (e.g. fireworks) or safety (e.g. airbags) applications, with others finding use in the defence industry. The range and specificity of applications is ever growing, and has led to considerable interest in the design of novel energetic materials. A particularly important parameter of energetic materials is their propensity to detonate on mechanical stimulation: impact, friction or shock. At present, novel energetic materials must first be synthesised in sufficient quantities for thorough experimental testing, with no *a priori* knowledge of its potential properties. This poses great safety concerns to developers, and is highly inefficient. Further, these methods are highly irreproducible and sometimes lead to erroneous conclusions.

In the present work we describe a physical mechanism to rationalise and predict the impact sensitivity of energetic materials. Based on knowledge of the effects of a mechanical impact, *ab initio* models are used to describe the processes of energy transfer within an energetic material. Within the model, consideration is given to the interplay between electronic and vibrational contributions to the detonation process. We discuss the identification of critical molecular motion that is required to initiate a thermal detonation. In doing so, we show that it is possible to simplify the problem of impact sensitivity, and consider only the role of vibrational energy transfer.

Within the framework of the model presented here, it becomes possible to begin to rationalise some structural features that are responsible for tuning impact sensitivity. These aspects will be introduced, alongside discussion of the role of co-crystallisation in modifying sensitivity parameters.

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An improved Energy-weighted density matrix embedding theory

In approaches such as dynamical mean-field theory (DMFT) the self-consistent optimization of a local fragment is performed using a hybridization with a true correlated environment. It was shown in Phys. Rev. B, 98, 235132 (2018) that using Energy-weighted Density Matrix Embedding Theory (EwDMET) the quantum fluctuations can instead be efficiently captured in a wave function perspective in a computationally cheap, frequency-independent, zero-temperature approach. It is discussed that the method has rigorous limits equivalent to existing quantum embedding approaches. We argue for the use of an alternate procedure for the technical aspect of hybridization construction EwDMET and provide analytical approaches to tackle the self consistency issue. We demonstrate this approach to solve the correlated dynamics of the Bethe lattice Hubbard model, as well as the one-dimensional Hubbard chain where we clearly show the benefits of this rapidly convergent description of correlated environmental fluctuations. We hope to demonstrate the approach for Hydrogen rings, where we efficiently embed an ab initio correlated chemical fragment wherein a quantitative accuracy is achieved despite only a single atom being explicitly treated.

DCMS MATERIALS 4.0 SUMMER SCHOOL

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Self-assembly of bis-salphen metal-organic frameworks

The recently-observed(1) self-assembly of salphen-based metal-organic frameworks (MOF) into networks of interconnected microrings with nano-thin strings may suggests a new intriguing tool for nanoscale patterning. However, the mechanism of this phenomenon yet needs to be clarified. In this work we will show how atomistic simulations help to shed light on supramolecular structure and details of the formation of this unusual self-assembly pattern.

We use ab initio calculations and all atomic molecular dynamics simulations in explicit together with umbrella sampling and free energy perturbation to investigate conformational space of the bis-salphen MOFs and potential self-assembly pathways. We observe that a particular conformation of the bis-salphen MOF allows it to form dimeric units, capable of linking with other units via either pi-pi or coordination Zn-O interactions in the two orthogonal directions. Due to these interactions bis-salphen MOFs can self-assemble into supramolecular chains, sheets and tubes, with highly variable mechanical properties. Furthermore, we show that the free energy gains of the two self-assembly pathways are determined by the solvent, which allows to control geometry of self-assembly and helps to relate our predictions to experimentally observed patterns. We propose(2) that the compounds under study form a 1D coordination polymer, the fibres of which are elastic enough to fold into toroidal globules upon solvent evaporation, while being able to link separate chains into extended networks. We also explain the separate roles of atomic groups, constituting the molecule and the way solvent controls the self-assembling structure. This opens an intriguing possibility to determine the mesoscale morphology of such molecular networks by tuning the functional groups of the molecule and macroscale parameters of the self-assembly process.

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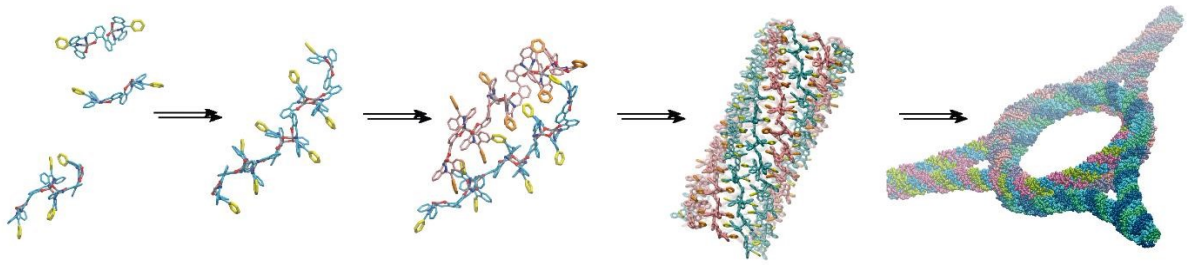

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Application of the CALPHAD method to additively manufactured steels

Selective Laser Melting (SLM) is a solid freeform fabrication process whereby a threedimensional part is built layer-by-layer by laser scanning over a powder bed. The high cooling rates achieved during solidification (~103-105 K/s) due to the small melt pool size, together with the effective heat conduction into the underlying layers are unique to the process. As the laser passes through a previously deposited material volume during deposition of neighbouring tracks and subsequent layers, the material experiences cyclic reheating in the form of a sequence of sharp temperature pulses up to temperatures close to the melting point with gradually decaying temperature. The complexity of the process and its non-equilibrium nature are responsible for the poor understanding of the underlying phenomena. This work outlines the possibilities and limitations of using the CALPHAD method to predict the microstructures obtained in commercial stainless steels by additive manufacturing.

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Excitons on two-dimensional topological insulators: Bi bilayers

Topological insulators present a novel feature, which is the presence of metallic edge states, as opposed to the bulk states which are insulating. This edge states have a fixed propagation direction, which may be exploited to force the dissociation of excitons, which are quasiparticles made of a bound electron-hole pair, thus generating an effective current. Since excitons can be produced by absorbing photons, this would constitute an alternative photovoltaic device. In this study we develop a tight-binding model with spin-orbit coupling to show first that Bi bilayers are topological insulators. Then, by turning on a Coulomb interaction in the system, we compute its exciton spectrum to see the contribution of the edge states.

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Temperature-induced phase transformations in Fe-C: Molecular dynamics approach

Carbon is the most important additive in steel productions and it significantly improves the mechanical response of iron. In polycrystalline body centered cubic iron, the mechanical behaviour under external loads is driven by the grain boundary character. Recent studies show that nanodiffusion of carbon leads to local adaptation of the material under external loads resulting in increased strength and deformability of iron. At a pressure of 13 GPa, iron transforms to a denser phase, called hexagonal closepacked phase (hcp). The transition pressure could be increased with carbon content because C atoms are trapped at local energy minima. So far, it is known that nanodiffusion of carbon in iron (bcc, fcc and hcp) is related to atomistic phenomena at the nanoscale and plastic deformation at the macroscopic scale. However, the diffusion of carbon under high pressure is not fully understood. First-principle theory is a powerful tool in condensed-matter physics. The objective of this project is to investigate the energetics of carbon diffusion in bcc, fcc and hcp iron by using the state-of-the-art DFT software CP-PAW and compare the result with other method like molecular dynamics.

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Extracting image orientation feature by using SVM classification

This poster introduces an support-vector-machine (SVM) method for extracting local orientation features from TEM images of dislocations. We generate 5000 synthetic dislocation images with random orientations and mark the orientations from 0 to pi with 30 categories. Based on synthetic dislocation images, an SVM model is built to predict the orientation. The resulting orientations can be further used to reconstruct the dislocations.

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Improving Porous TC4/UHMWPE Friction Spot Welding Joint Through Control of Welding Temperature and Force

Joining between metal and polymer has attracted significant attention recently due to its advantage of great weight reduction and excellent integrated physical/chemical properties. In this study, specially designed biomedical additive manufactured porous TC4 titanium alloy plate was successfully joined to ultra-high molecular weight polyethylene (UHMWPE) plate by friction spot welding (FSpW). The z-axial load (FZ) evolution has been measured with load cell, and welding temperature (TW) near TC4/UHMWPE interface has been measured with thermocouple. High tensile shear strength (~3000 N) has been realized through strong mechanical interlocking. Good macro-penetration of UHMWPE into TC4 porous structure (up to 80% filling rate) and sound micro-interlocking between metal and polymer were obtained. Relationship between TW/FZ and joint quality has been unveiled for the fabrication of defect-less joints. The research result has been successfully applied in the clinical application of temporomandibular joint prosthesis.

Keywords: Friction spot welding; Metal-plastic joining; Coupling effect; Additive manufacturing; Clinical application

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