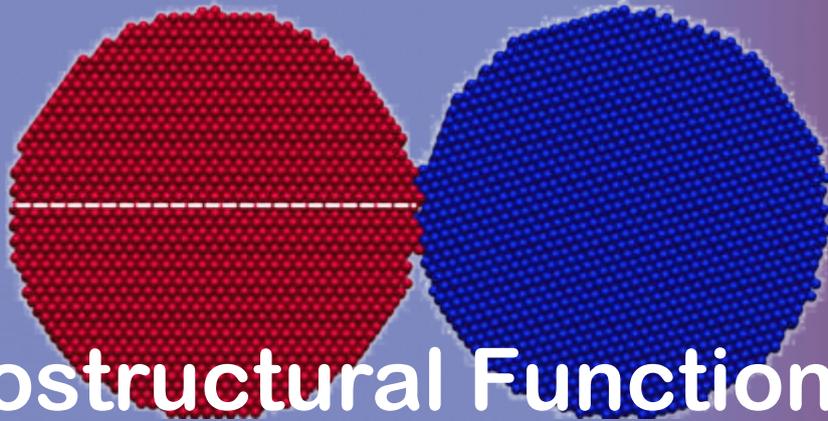
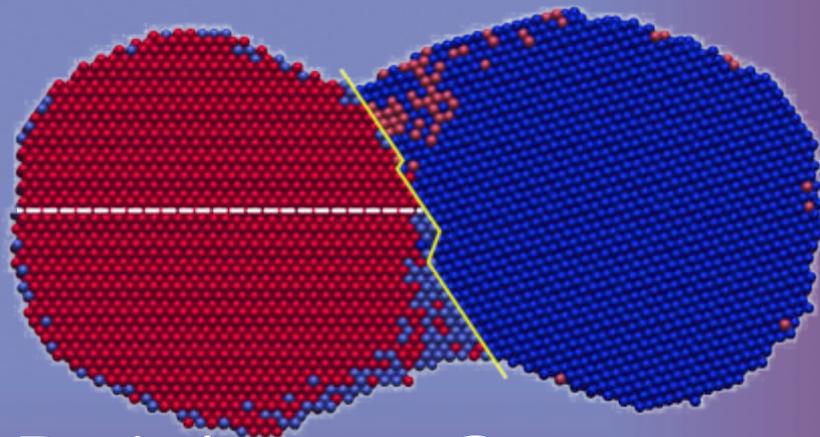


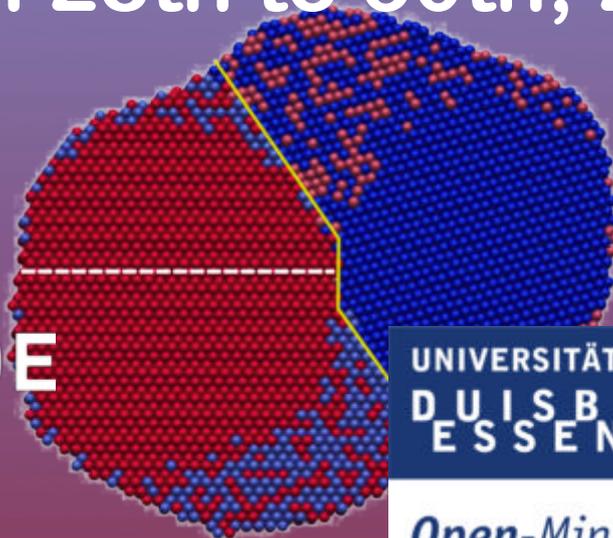
# MiFuN



Microstructural Functionality:  
Dynamics, Adaption, and Self-  
Healing at the Nanoscale



Duisburg, Germany  
April 28th to 30th, 2014



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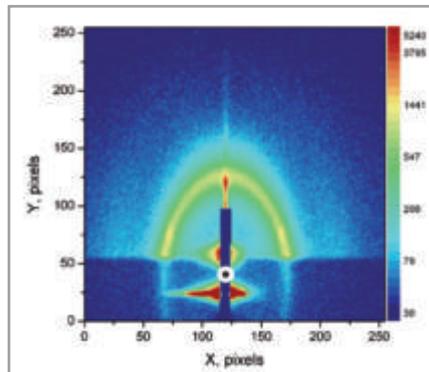
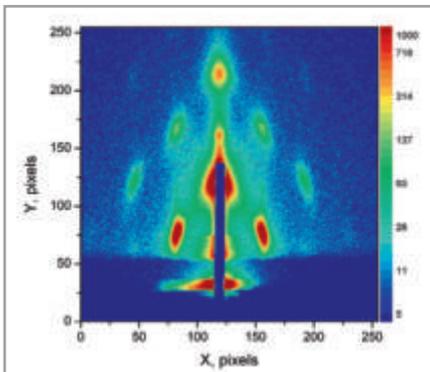
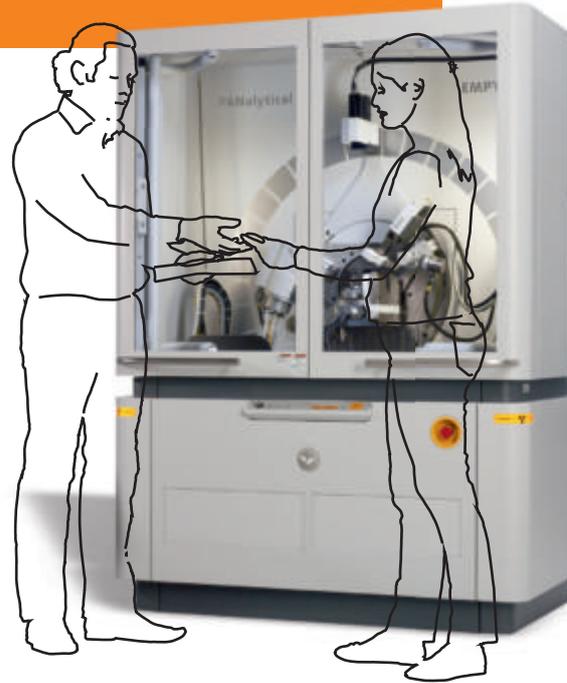
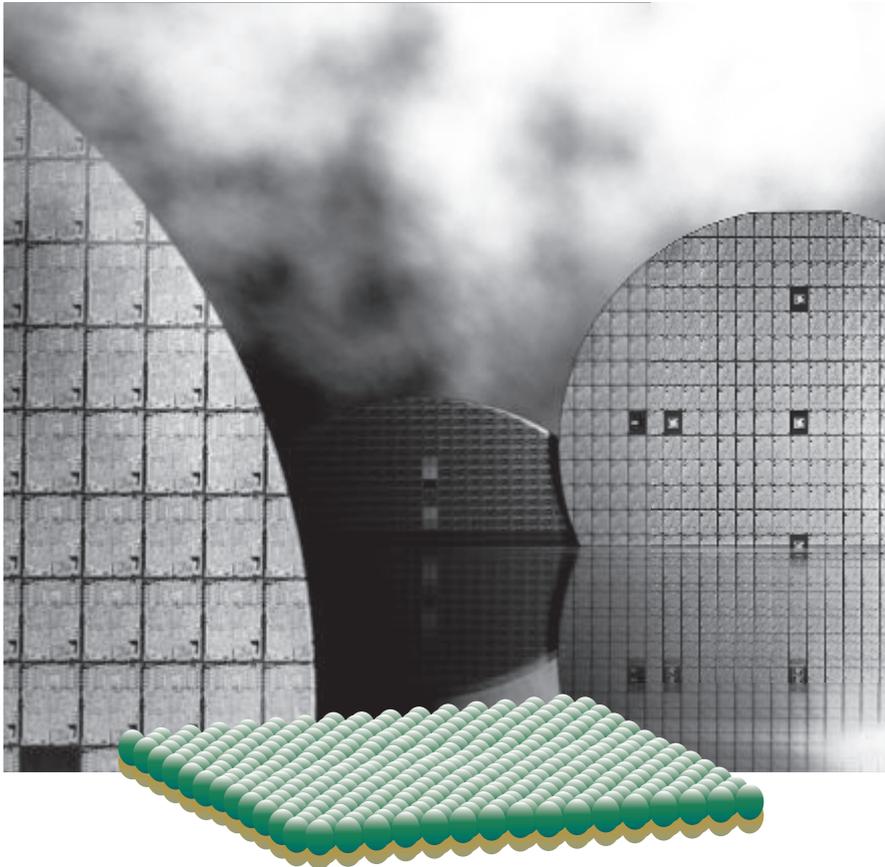
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# MiFuN

## Microstructural Functionality: Dynamics, Adaption, and Self-Healing at the Nanoscale

Duisburg, Germany, April 28th to 30th, 2014

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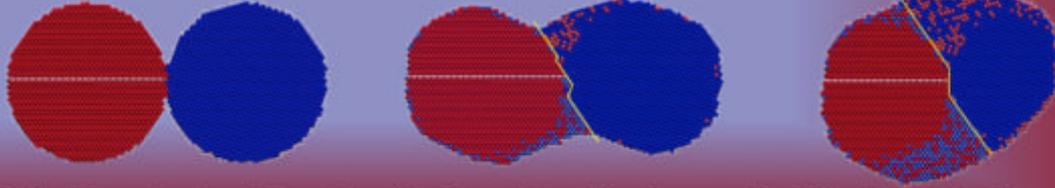
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# Program



MiFuN – Microstructural Functionality: Dynamics, Adaption, and Self-Healing at the Nanoscale



## Monday, April 28, 2014

08:00	<b>Registration</b>	
08:45	<b>Welcome</b>	Jörg Schröder
	<b>Switching and Tuning</b>	
09:00	<b>Horst Hahn, KIT</b> <i>Reversible tuning of materials properties by external fields</i>	chair: Gerd Bacher
09:45	<b>Rossitza Pentcheva, LMU München</b> <i>Control of metal-to-insulator transition in low-dimensional transition metal oxides: Insights from DFT+U calculations</i>	chair: Gerd Bacher
10:30	<b>Coffee Break</b>	
11:00	<b>Akihito Sawa, AIST, Tsukuba</b> <i>Interface type resistive switching in metal oxides</i>	chair: Marika Schleberger
	<b>Interfaces and Sintering</b>	
11:45	<b>Michael Moseler, U Freiburg</b> <i>Coarse graining and localized plasticity between sliding nanocrystalline metals</i>	chair: Marika Schleberger
12:30	<b>Lunch Break</b>	
13:30	<b>Labtours</b>	
	<b>Interfaces and Properties I</b>	
15:30	<b>Gregory Rohrer, Carnegie Mellon U</b> <i>Grain boundary energies, structural transitions, and their influence on microstructure</i>	chair: Markus Winterer
16:15	<b>Izabela Szlufarska, U Wisconsin</b> <i>Effects of grain refinement on friction and wear</i>	chair: Markus Winterer
17:00	<b>Coffee Break</b>	
17:30	<b>Michael Farle, U Duisburg-Essen</b> <i>Structure and composition-driven functionality in magnetic nanoparticles</i>	chair: Markus Winterer
18:15	<b>Informal Dinner</b>	



## Tuesday, April 29, 2014

08:30	Registration	
	<b>Phase Transitions and Self Organization</b>	
09:00	<b>Matthias Wuttig, RWTH Aachen</b> <i>Control on the nanoscale: Lessons to learn from phase change materials</i>	chair: Heiko Wende
09:45	<b>Winfried Petry, TU München</b> <i>From phonons to functionality</i>	chair: Heiko Wende
10:30	Coffee Break	
11:00	<b>Marcus Müller, U Göttingen</b> <i>Directing the self-assembly of copolymer materials</i>	chair: Axel Lorke
11:45	<b>Oliver Schmidt, IFW Dresden</b> <i>Elastic multifunctional nanomembranes: From concepts to applications</i>	chair: Axel Lorke
12:30	Lunch Break	
13:30	<b>Poster Session</b>	
	<b>Electromigration</b>	
15:30	<b>Dimitrios Maroudas, U Massachusetts Amherst</b> <i>Current-driven surface morphological stabilization and surface nanopatterning</i>	chair: Rolf Möller
16:15	<b>Kirk Bevan, McGill U</b> <i>The wind force and direct force in electromigration: a steady state perspective in the ballistic transport regime</i>	chair: Rolf Möller
17:00	Coffee Break	
17:30	<b>Frank Meyer zu Heringdorf, U Duisburg-Essen</b> <i>In situ investigations of electromigration in crystalline silver wires with defined grain-boundaries</i>	chair: Rolf Möller
18:15	Informal Dinner	

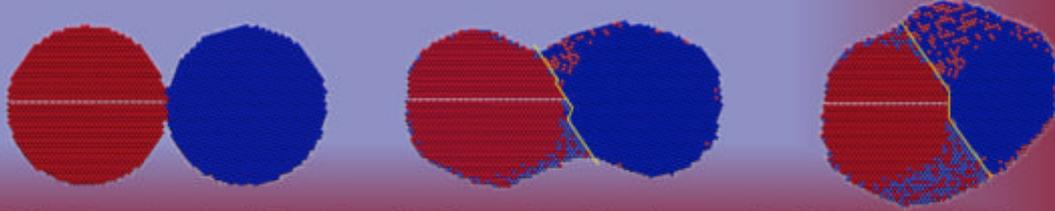


## Wednesday, April 30, 2014

08:00	Registration	
	<b>Interfaces and Properties II</b>	
08:30	<b>Karsten Albe, TU Darmstadt</b> <i>Grain boundary mediated plasticity of nanocrystalline and nanoamorphous metals: Insights from atomistic computer simulations</i>	chair: Peter Kratzer
09:15	<b>Gabi Schierning, U Duisburg-Essen</b> <i>Interfaces in thermoelectric materials</i>	chair: Peter Kratzer
10:00	Coffee Break	
10:15	<b>Ingo Steinbach, ICAMS, Bochum</b> <i>The influence of vacancy- and particle drag on coarsening in nanocrystalline metals</i>	chair: Bernhard Eidel
11:00	<b>Carl Krill, U Ulm</b> <i>Hipsters versus robber barons: The sociology of grain growth in a nanostructured world</i>	chair: Bernhard Eidel
	<b>Mechanical Properties and Self Healing</b>	
11:45	Lunch Break	
12:30	<b>Michel Barsoum, Drexel U</b> <i>Strain accommodation in kinking nonlinear elastic solids</i>	chair: Alfons Fischer
13:15	<b>Niels van Dijk, TU Delft</b> <i>Self-healing of structural damage in Fe-based alloys</i>	chair: Alfons Fischer
14:00	Coffee Break	
	<b>Outlook</b>	
14:15	<b>Martin Müser, FZ Jülich</b> <i>Modeling non-equilibrium dynamics at the nanoscale: Selected challenges and perspectives</i>	chair: Dietrich Wolf
15:00	<b>Joachim Mayer, RWTH Aachen</b> <i>Advanced TEM methods based on correction of the chromatic aberration</i>	chair: Dietrich Wolf
15:45	<b>Conclusion</b>	Markus Winterer
17:00 – 22:00	<b>Social Event and Conference Dinner</b>	



## Oral / Invited Presentations



MiFuN – Microstructural Functionality: Dynamics, Adaption, and Self-Healing at the Nanoscale

(In order of appearance in the oral program)

# Reversible tuning of materials properties by external fields

Horst Hahn\*

Institute for Nanotechnology and Helmholtz Institute Ulm, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The mechanical, physical and chemical properties of materials are determined by their microstructure. Modern materials science uses the complex interplay of defects, such as impurities, phases, point and line defects and interfaces, to tailor properties and obtain high-performance metallic alloys and ceramics. In this approach of materials design, properties can only be changed by modifying their microstructure, for example by initiating grain growth during annealing at elevated temperatures. Such a behavior, that fixes the properties irreversibly to the microstructure, is advantageous for many applications of materials, where long-term stability of the properties is required.

In contrast, tuning using external fields, i.e., electric, offers completely new opportunities for the fully reversible control of materials properties. Such tuning of physical properties will be demonstrated for several nanostructures, i.e. (epitaxial) thin films, nanoporous, nano particulate structures and nanowires. Tuning can be either achieved using dielectric/ferroelectric gating, well known from semiconductor physics, or by electrolyte gating using liquid or solid electrolytes. Furthermore, using electrochemical ion intercalation, fully reversible properties can be achieved. Finally, the concepts employed for tuning properties of nanostructures can be employed in applications as well. As an example, field-effect transistors based on inorganic nano particles as the channel material and solid electrolyte for the gating will be described.

**Notes**

# Control of metal-to-insulator transition in low-dimensional transition metal oxides: Insights from DFT+U calculations

Rossitza Pentcheva\*

Theoretical Physics, Faculty of Physics, University of Duisburg-Essen, Germany

Metal-to-insulator transitions (MIT) play a key role in condensed matter physics and materials science. Understanding the origin and control parameters of MIT is of ultimate importance for the development of next generation electronics devices. Material-specific density functional theory calculations can give valuable insights to uncover the underlying mechanisms.

In my talk I will address several cases: A variety of functional properties emerge at the polar LaAlO<sub>3</sub>/SrTiO<sub>3</sub>(001) interface. Here I will address finite size effects and the origin of a thickness-dependent MIT in LaAlO<sub>3</sub> films on SrTiO<sub>3</sub>(001) as well as its functionalization by oxide overlayers or metallic contacts [1-3]. As an example of dimensional confinement and strain-driven MIT I will discuss superlattices containing the correlated metal LaNiO<sub>3</sub> and the band insulator LaAlO<sub>3</sub> [4-6]. The presence of a surface and adsorbates influence significantly the charge order and trigger thereby a MIT at the Fe<sub>3</sub>O<sub>4</sub>(001) [7-8]. Finally, the influence of stoichiometry modulation and the resistive switching behavior in the layered compound in LanTnO<sub>3n+2</sub> will be elucidated [9].

Funding by the DFG SFB/TR80 and a grant for computational time at the Leibniz Rechenzentrum Garching are gratefully acknowledged.

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- [7] N. Mulakaluri, R. Pentcheva, M. Wieland, W. Moritz and M. Scheffler, *Phys. Rev. Lett.* **103**, 176102 (2009).
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**Notes**

# Interface type resistive switching in metal oxides

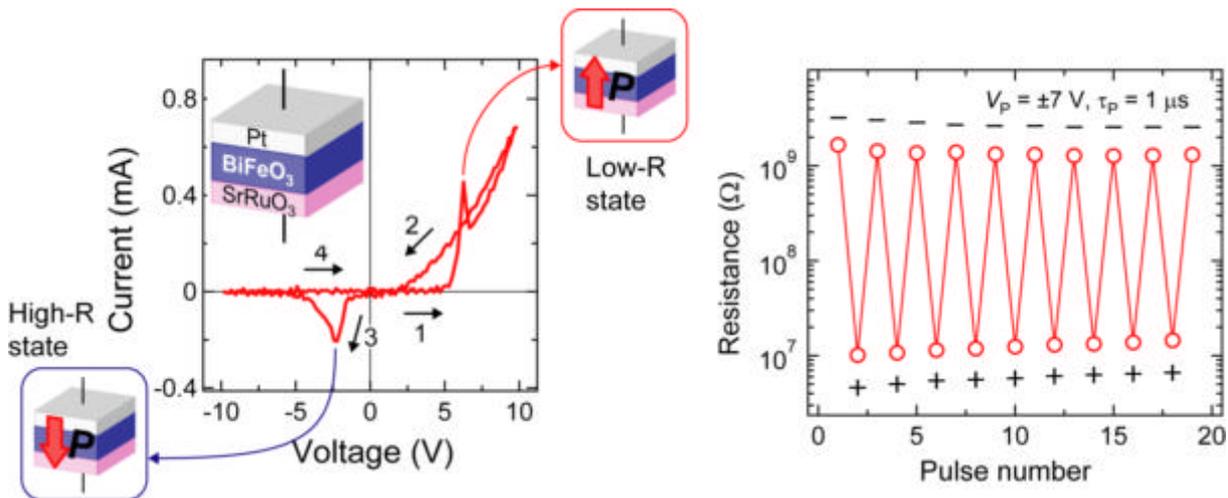
Akihito Sawa\*, Atsushi Tsurumaki-Fukuchi, Shutaro Asanuma, and Hiroyuki Yamada

National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Resistive switching phenomena in metal oxides have been intensively studied in the last decade, because of the potential for nonvolatile memory applications, i.e. resistance random access memory (ReRAM). Recent studies have revealed that the resistive switching phenomena is based on a nanoionic redox reaction triggered by Joule heating or electromigration of oxygen vacancies [1-3]. Since chemical alterations of materials are inevitably induced in both mechanisms, there is concern for the reliability, such as the data retention and endurance.

In the talk, we first review the representative models proposed for the driving mechanisms involved in the resistive switching phenomena [3], and then present our experimental results regarding interface-type resistive switching [3-6]. We have revealed that the valence change of the cations in metal-oxides induced by the electromigration of oxygen vacancies plays a crucial role for the mechanism of interface-type resistive switching [3,6]. Finally, we present our recent results of ferroelectric resistive switching memories consisting of  $\text{BiFeO}_3$  [7-10], in which resistive switching is caused by polarization reversal. We think that since the ferroelectric resistive switching memory is based on an electronic mechanism, it has an advantage over a conventional ReRAM in the reliability.

- [1] R. Waser and M. Aono, *Nat. Mater.* **6** (2007), 833
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**Fig. 1:** Current–voltage characteristics (left) and pulsed-voltage-induced resistive switching characteristics (right) of ferroelectric resistive switching memory  $\text{Pt}/\text{Bi}_{1-x}\text{FeO}_3/\text{SrRuO}_3$ . Arrows and numbers indicate the sequence of the hysteretic current loop.

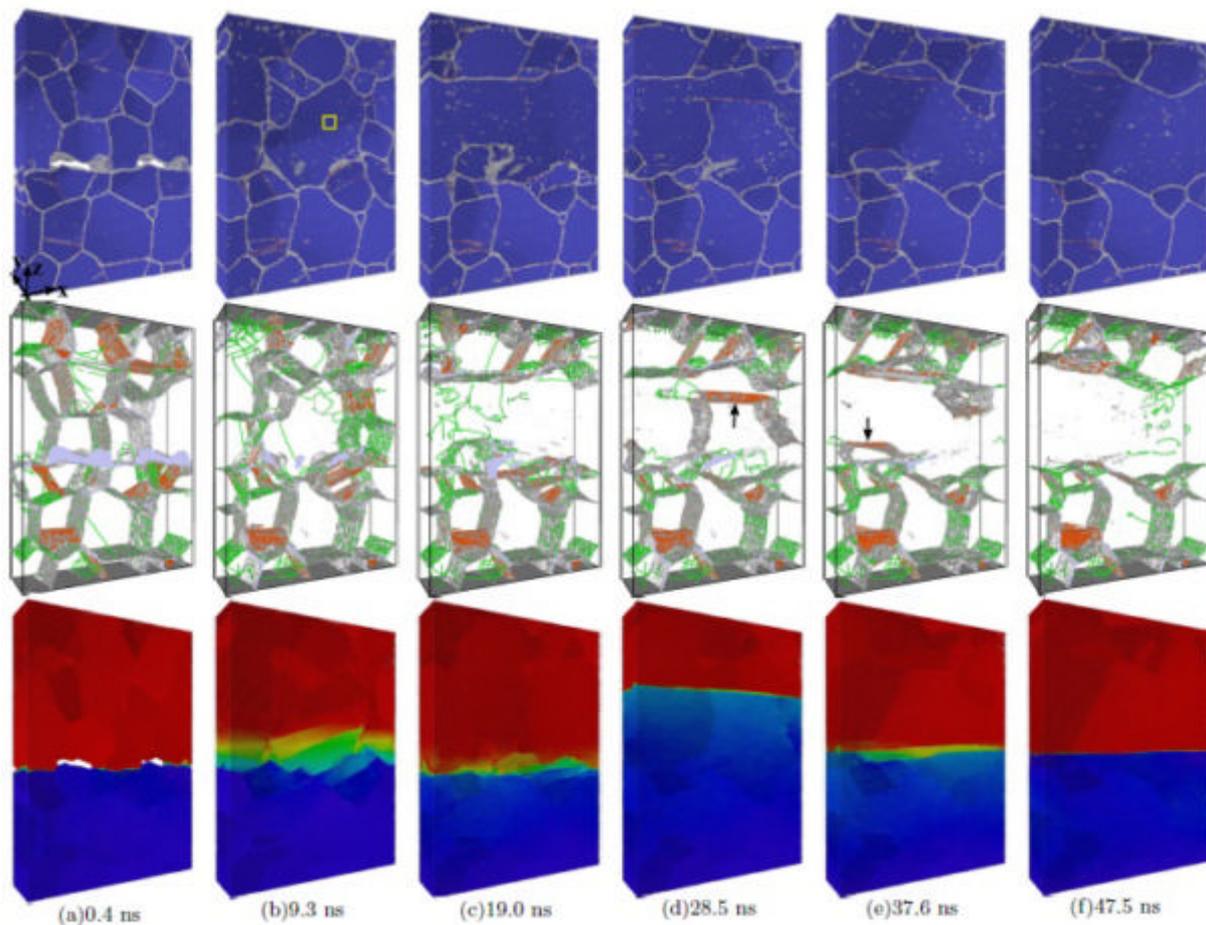
**Notes**

# Coarse graining and localized plasticity between sliding nanocrystalline metals

Pedro A. Romero, Tommi T. Järvi, Nils Beckmann, Matous Mrovec and Michael Moseler\*

Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Tribological shearing of polycrystalline metals typically leads to grain refinement at the sliding interface. In this presentation, however, it is shown that nanocrystalline metals exhibit qualitatively different behavior. Using large scale atomistic simulations, we demonstrate that during sliding, contact interface nanocrystalline grains self-organize through extensive grain coarsening and lattice rotation until the optimal plastic slip orientation is established. Subsequently, plastic deformation is confined to localized nano shear bands aligned with the shearing direction and emanating from voids and other defects in the vicinity of the sliding interface.



**Fig. 1:** Snapshots of the evolution of sliding contact between two nanocrystalline iron tribopartners. Each column presents the instantaneous state of the grain structure (top panels), the grain boundaries/dislocations (middle panels) and the corresponding sliding interface (bottom panels) at selected sliding times. The grain structure in the top row is exposed by perform a common neighbor analysis (CNA) (with blue/white/red standing for bcc/nonbcc/twin boundary atoms). The middle row shows the simultaneous state of the extracted dislocations and twin boundaries (with green/grey representing dislocations with  $1/2 < 111 > / \text{non } 1/2 < 111 >$  Burgers vectors and with gray/red marking the location of voids/twin boundaries). In order to correlate the structural dynamics with the velocity accommodation mode (i.e. the way the system distributes the sliding induced velocity gradient over the system), the strain rates are visualized in the bottom row by coloring the atoms according to their change in displacement along the sliding x-direction after every 0.2 ns on a scale from 0 (blue) to 1 nm (red). As sliding progresses, the counter bodies cold weld and establish a coarsened grain layer where plasticity concentrates and the sliding interface localizes.

**Notes**

# Grain boundary energies, structural transitions, and their influence on microstructure

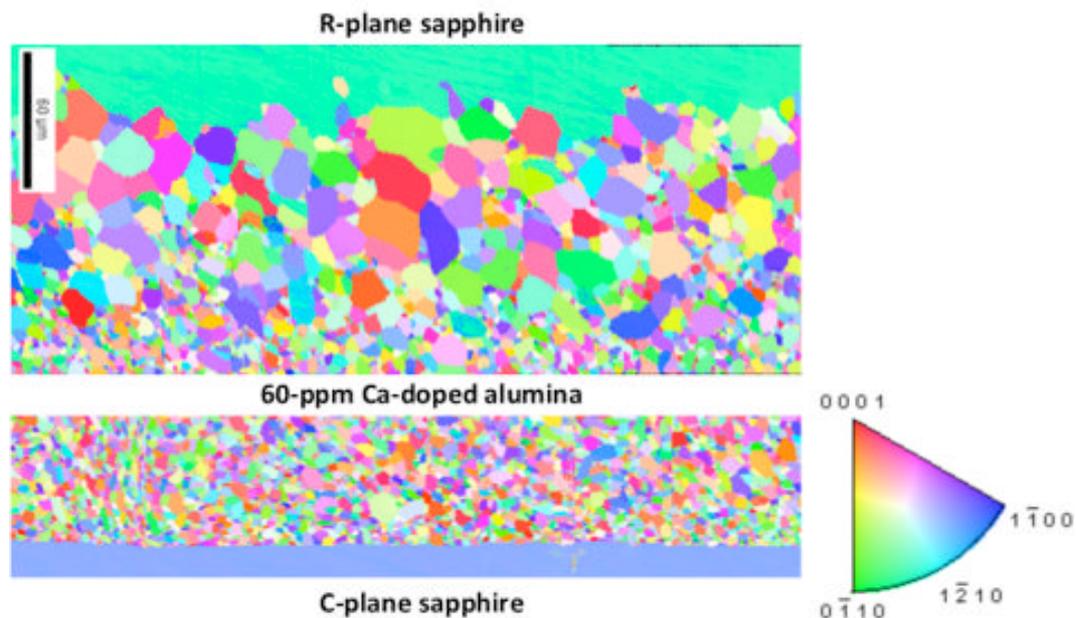
Stephanie A. Bojarski and Gregory S. Rohrer\*

Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, USA

The recent discovery that the structure and composition of grain boundaries can abruptly change, leading to discontinuous changes in grain boundary properties, such as energy and mobility, provides a key piece of information that helps to explain abnormal grain growth [1]. In this talk, I will first review experimental evidence that complexion transitions in bulk ceramics lead to a decrease in the grain boundary energy, using data from alumina and yttria [2-6].

As an example of recent research, I will describe experiments designed to test the effect of grain boundary energy on the nucleation of a transition from a low mobility to high mobility grain boundary complexion. These experiments employ novel samples consisting of yttria- and calcia-doped alumina sandwiched between two single crystals of sapphire. Grain boundary thermal groove measurements showed that the distribution of grain boundary energies at the single crystal-polycrystal interface is biased by the orientations of the sapphire crystals. Annealing above the critical temperature for the complexion transition showed that the high mobility complexion was more easily nucleated at the higher energy interface. The images in Fig. 1 show an example of one of the experimental outcomes, where grains near the higher energy interface have grown farther.

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**Fig. 1:** EBSD maps of a cross section of a sandwich sample after consolidation. On the left, a single crystal of sapphire with the R-plane in contact with 60 ppm Ca-doped  $\text{Al}_2\text{O}_3$ . On the right, a single crystal of sapphire with the C-plane in contact with the same 60 ppm Ca-doped  $\text{Al}_2\text{O}_3$ . The grains are colored by their orientation perpendicular to the plane of the image, according the legend to the right.

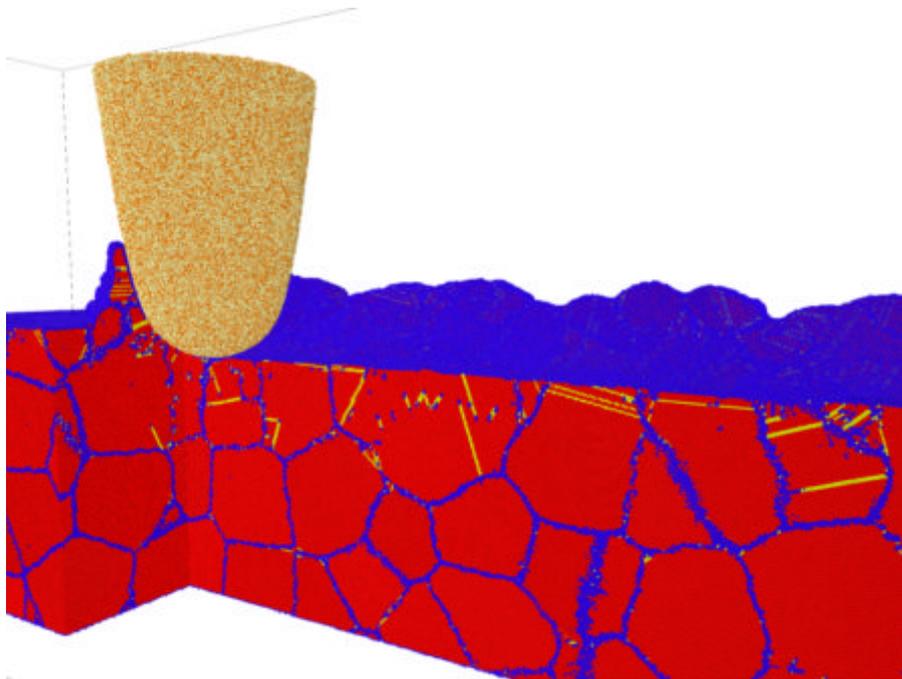
**Notes**

# Effects of grain refinement on friction and wear

Izabela Szlufarska,\* Ao Li, Maneesh Mishra

Department of Materials Science & Engineering, University of Wisconsin – Madison, Madison, USA

It has been estimated that about one third of energy produced in industrialized countries is lost to overcoming friction. In this talk we will discuss a promising pathway for design of coating materials with superior tribological properties, which is by grain refinement to the nanometer regime. We will discuss the effects of grain refinement on friction and wear in both ceramics and metals, using SiC and Cu (Fig. 1) as representative materials. For both classes of materials, we identify the dominant deformation mechanisms and demonstrate new size effects in deformation. For ceramics, reduction of grain size leads to suppression of fracture and the dominant wear mechanism becomes grain boundary sliding and grain pull-out. For metallic system we find that the mechanisms are strongly coupled to the contact size and that there is an optimum coupling between the internal length scale (grain size) and the external length scale (contact size) that minimizes the rate of material removal. These findings provide new tools for microstructural design of wear-resistant coatings.



**Fig. 1:** Molecular dynamics simulations of plowing of nanocrystalline Cu using a rigid SiC tip. The average grain diameter in the sample shown here is 15 nm.

**Notes**

# Structure and composition-driven functionality in magnetic nanoparticles

Michael Farle\*

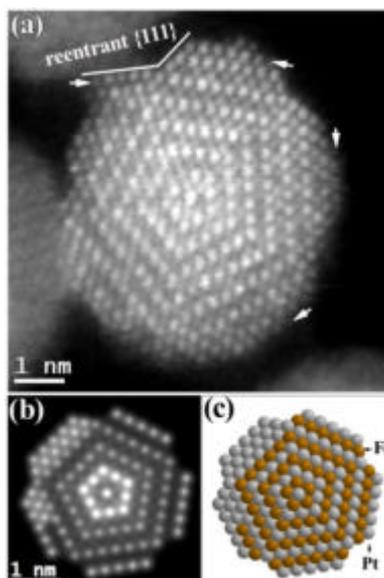
Experimental Physics, Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany

The hysteresis and magnitude of the magnetization of a magnet like a single ferro- (superpara-) magnetic nanoparticles is determined by its morphology, shape, composition, and crystal structure [1,2]. In nanoparticles competing energies known also for bulk systems originating from strain, chemistry, surface and defects change their relative importance and new structures become stable or at least metastable. Such structures can stabilize magnetic properties which cannot be achieved in volume materials and open new routes to tailoring magnetism for innovations in energy related materials (Rare-Earth free permanent magnets) and processes (spin logic) as well as in biomedical applications.

In this talk I will review some examples illustrating the sensitivity of magnetic properties to strain, surface and also intraparticle interface effects between surface (shell) layers and the core: 1) 'Enhanced' magnetism in Co nanoparticles due to the formation of oxidic shells [3,4] and the formation of nanocapsules by the Kirkendall effects. 2) The ageing effects in FeAg dumbbell particles [5], 3) Strain and surface effects leading to a loss of hard-magnetic properties in bimetallic FePt nanoparticles (Fig. 1) [6,7]. It is demonstrated that many 'new' properties detected in nanoparticles can be understood by referring to classical textbook-like crystal field effects in magnetism.

Work performed within the framework of EU- networks SyntOrbMag, IMAGINE and the DFG,SFB 445.

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**Fig. 1:** (a) Experimental high-resolution HAADF (Z-contrast) image of a chemically-ordered decahedral FePt NP. Brighter spots correspond to heavy Pt atomic columns ( $Z=78$ ) while less bright spots correspond to Fe columns ( $Z=26$ ). The white arrows indicate Pt-enriched surfaces which contain only few atoms in the column. (b) HAADF simulation of an ordered decahedral FePt NP according to the atomic model of ordered decahedral FePt shown in (c). Taken from Ref. [6].

**Notes**

# Control on the nanoscale: Lessons to learn from phase change

Matthias Wuttig\*

Physics of Novel Materials, RWTH Aachen University, Aachen, Germany

Phase change media are among the most promising materials in information technology. These materials can be very rapidly switched between the amorphous and the crystalline state, indicative for peculiar crystallization behaviour. They are already employed in rewriteable optical data storage, where the pronounced difference of optical properties between the amorphous and crystalline state is used. This unconventional class of materials is also the basis of a storage concept to replace flash memory.

This talk will discuss the unique material properties which characterize phase change materials. In particular, it will be shown that the crystalline state of phase change materials is characterized by the occurrence of resonant bonding, a particular flavour of covalent bonding [1]. This insight is employed to predict systematic property trends [2] and to develop non-volatile memories with DRAM-like switching speeds potentially paving the road towards a universal memory [3]. Phase change materials do not only provide exciting opportunities for applications including 'greener' storage devices, but also form a unique quantum state of matter as will be demonstrated by transport measurements [4,5]. In addition, they demonstrate remarkable crystallization kinetics. Successful application of these materials requires control of structure formation on the nanometer length and nanosecond time scale. Our understanding of the control mechanisms, which can be utilized here, will be presented.

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**Notes**

# From phonons to functionality

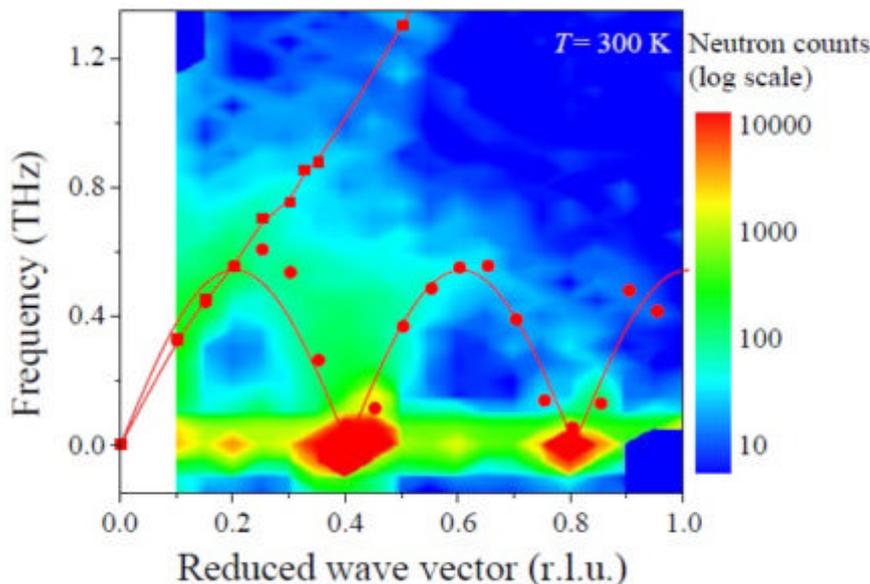
Winfried Petry\*

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Why do by far most of the elemental metals condense in the open bcc structure? And how is this related to the self diffusion in bcc metals? Phonon spectroscopy with thermal neutrons explores the harmonic and anharmonic interatomic potentials, thereby revealing the importance of lattice entropy in stabilizing the high temperature structures, and showing how atomic diffusion as the most anharmonic event one can think of follows trajectories along lowest lattice potentials.

Iron as base element of many work pieces and rich in phase transitions will serve as first example for bridging from phonons to functionality. Classical shape memory alloys like NiTi and more advanced ferromagnetic shape memory alloys like Ni<sub>2</sub>MnGa will serve as further example for demonstrating the importance of interatomic potentials for understanding and designing functionality.

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**Fig. 1:** Phonon dispersion in Ni<sub>2</sub>MnGa, showing the extremely low lying acoustic phonons for the 5M modulated and tetragonal distorted martensitic phase.

**Notes**

# Directing the self-assembly of copolymer materials

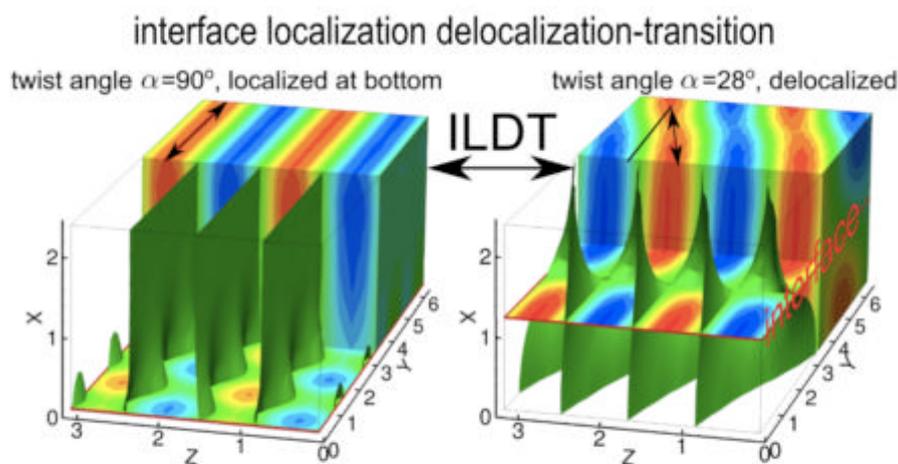
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Copolymers are flexible macromolecules that are comprised of two (or more) blocks. The incompatibility between the constituents of different blocks gives rise to microphase separation on the length scale of 5 - 70 nm. Much effort has been devoted to utilizing these soft materials as templates for nanostructures, e.g., for integrated circuits and memory devices, and fabricating defect-free structures or structures that differ from the thermodynamically stable morphologies in the bulk.

Computational modeling can contribute to optimizing material parameters such film thickness, interaction between copolymer blocks and substrate, geometry of confinement, and it provides fundamental insights into the physical mechanisms of directing the self-assembly, addressing both the equilibrium structure and thermodynamics and the kinetics of self-assembly. I will discuss highly coarse-grained models that allow us to access the long time and large length scales associated with self-assembly [1,2], review computational methods [2,3] to determine the free energy of self-assembled structures [4,5] and to investigate the kinetic pathways of structure formation [6]. Opportunities for directing the kinetics of self-assembly by temporal changes of thermodynamic conditions will be discussed.

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**Fig. 1:** Morphology of a lamella-forming block copolymer film sandwiched between two stripe-patterned solid substrates whose patterns are twisted by an angle,  $\alpha$ . In the left panel the twist grain boundary between domains that are aligned with the respective substrate patterns is localized at the bottom substrate, whereas it is fluctuating around the center of the film in the right panel. From [4]

**Notes**

# Elastic multifunctional nanomembranes: From concepts to applications

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Nanomembranes are thin, flexible, transferable and can be shaped into 3D micro- and nanoarchitectures. This makes them attractive for a broad range of applications and scientific research fields bridging from flexible magnetoelectronic devices to ultra-compact autonomous microrobotic systems. If nanomembranes are differentially strained they deform themselves and roll-up into tubular structures upon release from their mother substrate. Rolled-up nanomembranes can be exploited to rigorously compact electronic circuitry, energy storage units and novel optical systems. An ambitious idea is to create massively parallel and fully integrated lab-in-a-tube systems on a single chip, which can stimulate, sense, analyze and process biomaterials in minute volumes. If appropriate materials are chosen, rolled-up tubes act as tiny catalytic jet engines which in the ultimate limit may drive compact multifunctional autonomous systems for medical and environmental applications. The elastic response of nanomembranes to in- and extrinsic stimuli is decisive to explore novel sensing and actuation concepts.

**Notes**

# Current-driven surface morphological stabilization and surface nanopatterning

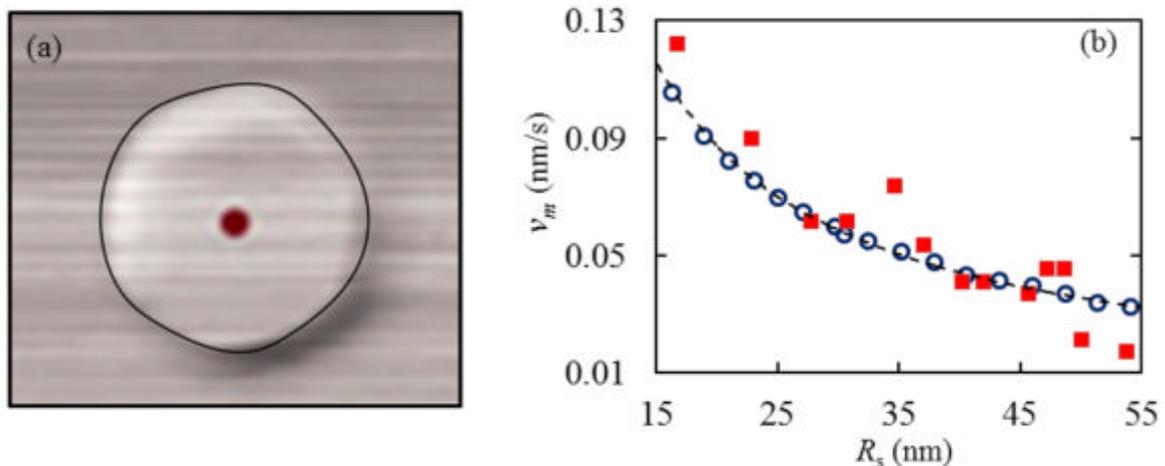
Dwaipayan Dasgupta, Georgios I. Sfyris, Lin Du, and Dimitrios Maroudas\*

Department of Chemical Engineering, University of Massachusetts, Amherst, USA

Externally applied fields, such as electric fields and temperature gradients, can be used to drive the morphological evolution of surfaces of crystalline solids. We have studied the use of such external fields to prevent surface morphological instabilities in stressed solids and to drive the assembly of single-layer epitaxial islands. Toward this end, we examine the surface morphological stability of electrically and thermally conducting crystalline elastic solids in uniaxial tension [1-3] and of biaxially coherently strained epitaxial films on substrates [4] under the combined action of an electric field and a temperature gradient. We use linear stability theory and self-consistent dynamical simulations based on a surface mass transport model that accounts for surface electromigration and thermomigration induced by the applied electric field and thermal gradient, respectively, surface diffusional anisotropy, and the temperature dependence of surface diffusivity. We find that properly directed external fields of magnitude higher than a critical value can stabilize the planar surface morphology and derive the conditions for synergistic action of the external fields, as well as the criticality conditions for surface stabilization.

We have also developed and validated a nonlinear model for the current-driven dynamics of single-layer epitaxial islands on crystalline substrates (Fig. 1) [5]. Simulations based on the model show that the dependence of the stable steady island migration speed  $v_m$  on the inverse of the island size is not linear for larger-than-critical island sizes [5]. In this nonlinear regime, we report morphological transitions, Hopf bifurcations, and instabilities for various surface crystallographic orientations and island misfit strains [5]. Moreover, we have studied the evolution of pairs of different-size islands driven to coalescence and explored the effects of three key geometrical parameters: the sizes of the two islands of the pair and their center-to-center line misalignment with respect to the electric-field direction [6]. We discovered various patterns ranging from equal- and different-size stable steady island-pair configurations to many-island patterns that can be tailored by controlling the initial-pair geometrical parameters and the duration of application of the electric field.

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**Fig. 1:** Comparison of simulation predictions with (a) experimental observations of island morphology and (b) experimental data (solid red squares) for the dependence of the island migration speed,  $v_m$ , on the island radius,  $R_s$ , during current-driven migration of morphologically stable single-layer homoepitaxial islands on Ag(111). Simulation results: (a) solid line and (b) open blue circles.

**Notes**

# The wind force and direct force in electromigration: a steady state perspective in the ballistic transport regime

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Electromigration has gained increased prominence in recent years, due to the shrinking footprint of nanoelectronic devices [1]. Smaller semiconductor devices require smaller interconnects with a greater surface to volume ratio and correspondingly higher current densities. This leads to increased electromigration and lower inherent reliability [1]. To mitigate electromigration and improve reliability, an improved understanding of electromigration is needed [2].

In this talk, an alternate perspective on the electronic force driving nanoscale electromigration is provided [2,3,4,5]. Starting from first-principles within the Landauer-Buttiker transport picture, the nature of the wind force and direct force in electromigration is explored from the 'bottom-up' [3,4,5]. From this inquiry we are lead to the intriguing conclusion that the wind force and direct force are essentially the same in the ballistic limit [4]. The results of this study aim to stimulate new discussion in this field, in urgent need of fresh ideas to address the growing electromigration problem in semiconductor interconnects [1,6].

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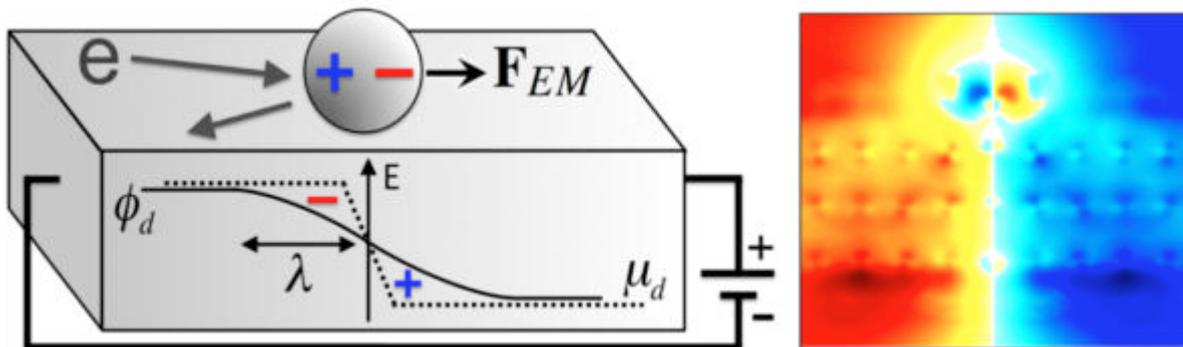


Fig. 1: Electromigration and the voltage drop

**Notes**

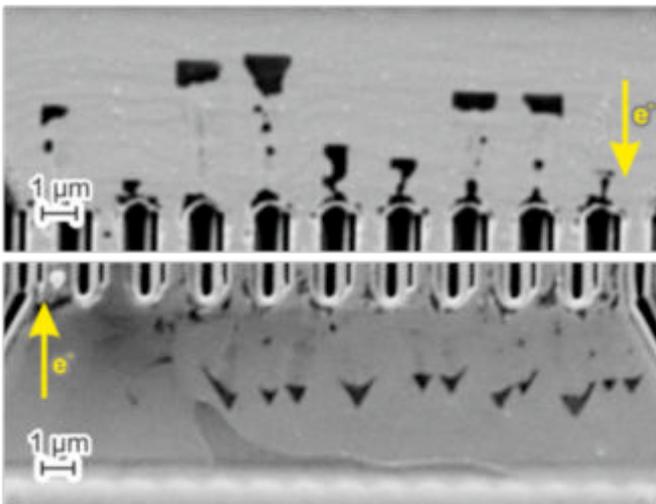
# In-Situ investigations of electromigration in crystalline silver wires with defined grain boundaries

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Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany

Electromigration effects in poly-crystalline metallization layers strongly limit the performance in today's semiconducting circuits. With smaller active areas in such devices, interconnects are shrinking as well, changing the surface-to-volume ratio so that surface transport becomes increasingly important. Similarly, with smaller interconnects, the influence of single grains on the electromigration becomes an important issue, as ultimately, the wires will only be one grain wide (with grain boundaries only perpendicular to the current direction). We use well controlled bi-crystalline Ag test structures [1,2] to study the interaction of electromigration driven voids with the crystal lattice by in-situ scanning electron microscopy (SEM). We find that the shape of propagating voids is strongly influenced by the lattice symmetry [2,3]. In (111) oriented areas of the test-structures we predominantly find triangular shapes, while in (001) oriented regions we find rectangular shapes. In the motion path of voids we observe an increased number of additional voids (void traces) [4]. Upon reversing the electrical current direction, voids also follow these void traces.

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**Fig. 1:** Electromigration-caused voids with a (top) square shape in the (001) part of a Ag test structure and a (bottom) triangular shape in the (111) part of a Ag test structure.

**Notes**

# Grain boundary mediated plasticity of nanocrystalline and nanoamorphous metals: Insights from atomistic computer simulations

Karsten Albe\*, Jonathan Schäfer, Alexander Stukowski, Tobias Brink, Yvonne Ritter, Daniel Sopus

FG Materialmodellierung, FB Material- und Geowissenschaften, TU Darmstadt, Darmstadt, Germany

The active deformation mechanisms governing the plastic behavior of nanocrystalline (nc) metals and alloys strongly depend on grain size and strain rate and are distinct from coarse grained materials. Although it is well known that grain boundaries play a key role for the deformation behaviour of nc-metals, very little is known, however, how the mechanical properties of alloyed nanocrystals are affected by the presence of solutes.

In this contribution, hybrid Monte-Carlo and molecular dynamics simulations of various miscible alloys will be presented, which provide clear evidence that the plastic deformation of nc alloys is the result of a delicate interplay between compositional dependent, dynamic grain boundary effects and bulk properties. Examples are shown for grain boundaries that undergo irreversible changes under deformation that can be quantified by an excess enthalpy. Comparison with recent experimental results from calorimetry provides an astonishing agreement between predictions from computer simulations [1-5]. In the second part of the presentation the existence of nanoglasses is discussed, which have been postulated in the early nineties in analogy to nanocrystals by Gleiter et al.. It is shown that even in disordered amorphous metals glass-glass interfaces can be introduced, which are characterized by a modified short-range order and an excess volume. Thus, we postulate that in analogy to crystalline materials even in amorphous metals the properties can be tuned by varying microstructural features [6-8].

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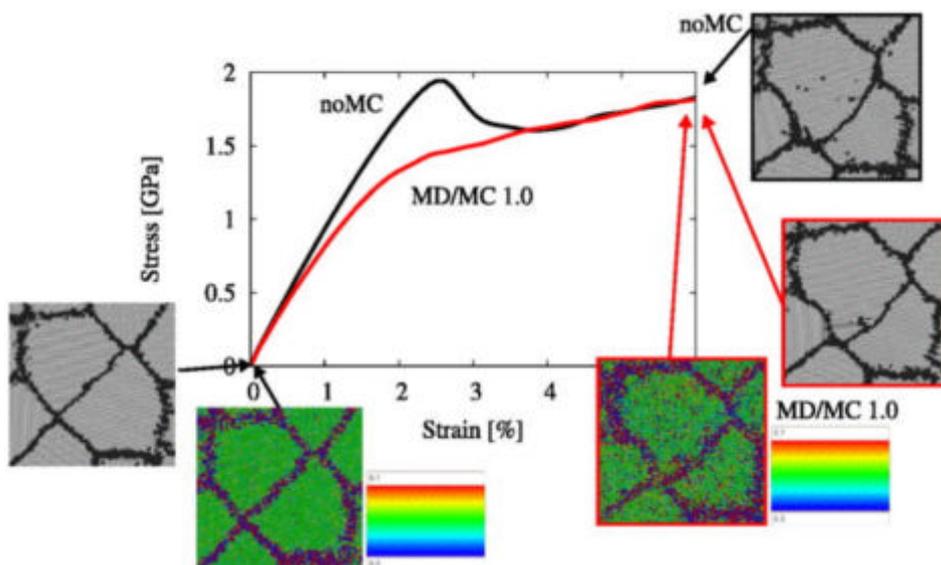


Fig. 1: MD/MC simulation of Pd-Au (50%) under tensile load [3].

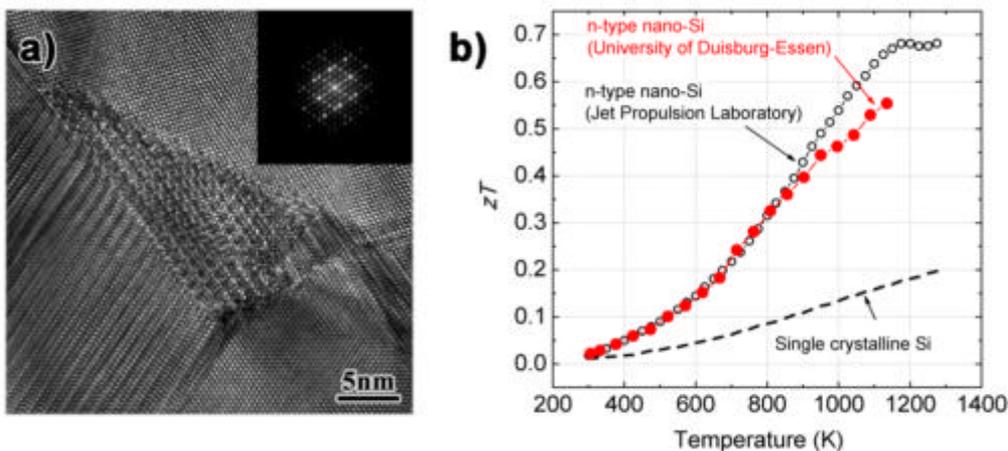
**Notes**

# Interfaces in thermoelectric materials

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Thermoelectric generators (TEGs) convert heat fluxes directly into usable electrical energy. For this, materials with a high thermoelectric figure of merit,  $zT = \alpha^2 \sigma T / \kappa$ , with Seebeck coefficient  $\alpha$ , electrical conductivity  $\sigma$ , thermal conductivity  $\kappa$ , and temperature  $T$  are needed. With an increasing understanding of the interrelation between the involved transport coefficients, thermoelectric materials have been greatly improved during the last decade. One of the most versatile approaches towards a figure of merit optimization has been nanostructuring and nowadays also materials which perform poorly in their single crystalline form as for instance silicon, can have competitive performance as nanocrystalline materials. The interfaces within the material reduce the lattice thermal conductivity by scattering the heat carrying phonons effectively. Further, often an increase of the Seebeck coefficient of the nanomaterial has been reported. If the mobility of the electrons is only moderately affected, the nanostructure is effective in improving the overall thermoelectric efficiency. But the role of the interfaces for the electronic and phononic transport has not yet been fully revealed. Some open questions, which will be discussed (but not answered) in this contribution, are: i) Why is the Seebeck coefficient of nanocrystalline materials sometimes increased compared to the Seebeck coefficient of a comparably doped polycrystalline material? ii) Some interfaces are transparent for electrons while other lead to a decrease of the electrical conductivity. While it is clear that the atomic structure at the interface will influence the local electronic structure, it is unclear how the interface modifies the electron phonon coupling, which also plays an important role on the electrical conductivity. iii) What is the mechanism and influence of atomic structure on the reduction of thermal conductivity at a grain boundary? The standard models for interpretation of an interface resistance are the acoustic and diffuse mismatch models. They have been derived from and tested against highly idealized interfaces which carry little resemblance with a grain boundary in a realistic material.



**Fig. 1:** a) High resolution TEM image of a typical grain structure of a nanocrystalline bulk silicon, TEM courtesy of R. Theissmann. b) Figure of merit,  $zT$ , of nanocrystalline bulk silicon from different groups.

**Notes**

# The influence of vacancy- and particle drag on coarsening in nanocrystalline metals

Reza Darvishi Kamachali, Christian Schwarze and Ingo Steinbach\*

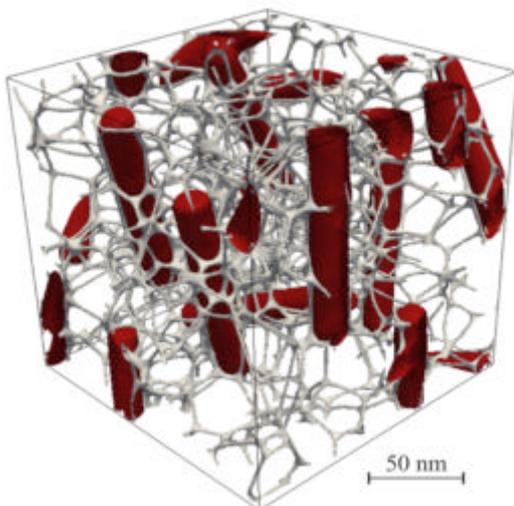
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Bochum, Germany

Retardation of grain growth is important to maintain the excellent mechanical properties of nanocrystalline metals. We discuss vacancy and particle drag on grain boundaries using a mesoscopic phase-field model implemented in the open source software OpenPhase [1].

Vacancies are mobile point defects which are associated by small amounts of volume causing distortion in the presence of stress gradients. Since grain boundaries act as sources or sinks of vacancies this is a significant issue in nano-materials with large amount of grain boundaries. A model for the interdependency between vacancy diffusion and evolving stress gradients around the grain boundaries is developed and applied to study grain growth on the nanoscale [2-4]. We have found that two competitive processes, namely curvature-driven motion of grain boundaries and stress-driven vacancy diffusion cause slow nanograin growth regime with a continuous extension to normal grain growth.

Secondly carbon-nanotubes and other inclusions are discussed as agents to suppress grain growth at the nano scale, e.g. in the aluminium alloys [5]. In our phase-field studies [6] we investigate Zener drag and pinning and have shown that the unique shape of CNTs makes their pinning behaviour to be configuration dependent. Large-scale simulations are done to investigate effect of size and distribution of CNTs on the grain growth (Fig. 1). We also investigate stability of grain boundaries in contact with CNTs.

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**Fig. 1:** Extracted volume of large-scale three-dimensional simulation with cylindrical particles (CNTs): length: 100 nm, radius: 7.5 nm, volume fraction: 4 vol.%. Grey lines are triple junctions or junctions of higher order.

**Notes**

# Hipsters versus robber barons: The sociology of grain growth in a nanostructured world

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Rainer Birringer  
FR 7.2 Experimental Physics, University of the Saarland, Saarbrücken, Germany

Just like our own world, the nanoworld is far from an egalitarian place. Never is this more obvious than during grain growth – the unbridled battle between crystallites for dominance in an economy based not on the capitalistic exchange of money in return for goods and services but on stochastic swaps of atoms biased by the invisible hand of thermodynamics. This process is essentially a war of attrition, culminating in the triumph of a select few over all the rest. What characteristics separate the winners from the losers in this bitter struggle for survival? Paradoxically, two diametrically opposed growth strategies seem to impart the best chance for ultimate success:

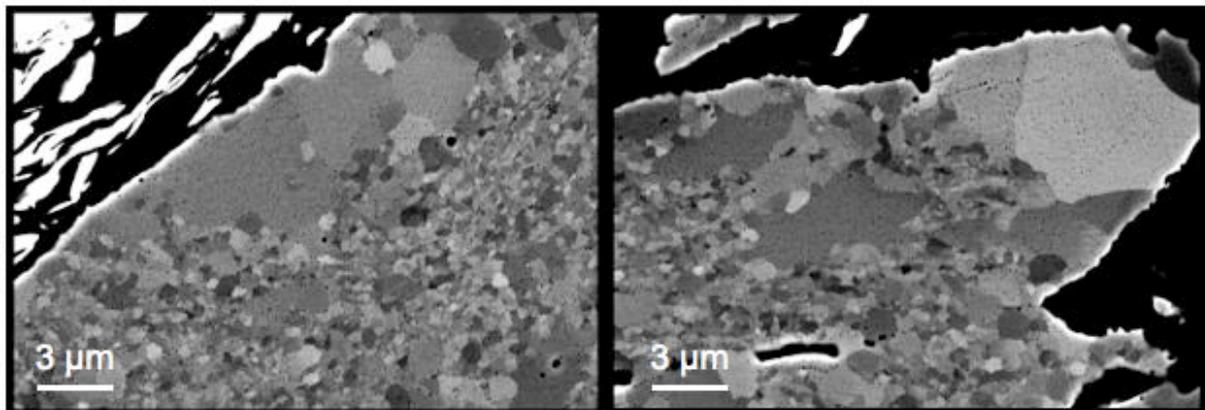
- 1) Feigned disinterest in growth, allowing the other grains to fight it out among themselves, while surreptitiously profiting from their losses;
- 2) Relentless aggression, voraciously appropriating atoms from neighboring grains at the fastest rate possible.

All grains follow Strategy #1 during so-called normal grain growth, but if only one grain drops its pretense of pacifism, then abnormal grain growth ensues, and Strategy #2 is by far the better plan. Perhaps not surprisingly, studies find that abnormal grain growth is common to a variety of nanocrystalline materials, regardless of composition or synthesis route.

In an effort to lower the tensions between warring crystallites, one can deliberately add an atomic species known to segregate to the grain boundaries, thereby reducing both the driving force for grain growth and the mobility of the boundaries themselves. But even this approach is limited in its capacity to improve the thermal stability of the nanocrystalline state: once grain growth commences, it overwhelms the peace-keeping forces in certain regions of the sample, leading to highly bimodal grain size distributions (Fig. 1) [1]. Even more striking is the room-temperature grain growth observed in high-purity nanocrystalline materials like Pd [2]. Coarsening is abnormal in this case, as well, but with an unusual twist: the aggressors rapidly take on a fractal morphology that is reminiscent of cluster shapes generated by percolation processes! Using a modified phase-field algorithm, we have tested whether such fractal abnormal grain growth can be modeled as the manifestation of opportunistic percolation along a grid defined by the initial ensemble of nanometer-sized grains. The right combination of robber baron and hipster mentalities is found to reproduce the fractal dimensionality observed in experiment.

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**Fig. 1:** Bimodal grain size distribution in nanocrystalline Fe<sub>95</sub>Ti<sub>5</sub> annealed at 1100°C for 1 h.

**Notes**

# Strain accomodation in kinking nonlinear elastic solids

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A decade ago we have identified a huge class of solids that we termed kinking nonlinear elastic, KNE, because one of their important – and in many cases only - deformation mode is the formation of fully and spontaneously reversible, dislocation-based incipient kink bands, IKBs. Compelling evidence, obtained from simple compression, in situ neutron diffraction, and nanoindentation experiments will be presented that show that KNE solids include the MAX phases, most hexagonal metals, layered silicates such as mica, sapphire, graphite, ZnO and LiNbO<sub>3</sub>, among many others. IKBs allow materials with only two independent slip systems – i.e. basal slip - an extra degree of freedom in strain accomodation, that can be fully and spontaneously reversible, while dissipating significant amounts of energy due to the to-and-fro motion of the dislocations involved. Lastly we claim that most solids with  $c/a$  ratios  $> 1.5$  - which per force are plastically anisotropic – can, if they do not twin first, deform by reversible kinking. It follows that KNE play a much more important role in our daily life than has hitherto been appreciated.

**Notes**

# Self-healing of structural damage in Fe-based alloys

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<sup>2</sup> Aerospace Engineering, Delft University of Technology, Delft, The Netherlands

Fe-based alloys can exhibit premature creep fracture, which arises from the formation, growth and coalescence of nano-scale cavities and cracks. Self-healing is a promising new approach to prevent damage growth by nano-scale precipitation on the creep cavity surface.

To explore the potential self-healing of open volume defects by precipitation, we studied the defect-induced high temperature precipitation behavior in Fe-Cu and Fe-Cu-B-N [1-3] and Fe-Au and Fe-Au-B-N [4-6] alloys by several nano-scale techniques including electron microscopy, positron annihilation spectroscopy and small-angle neutron scattering. The site-specific Cu and Au precipitation at dislocations and along grain boundaries demonstrates that these solute atoms act as efficient self-healing agents in the ferrous matrix. It is found that Au has a significantly higher preference to precipitate at defect sites than Cu, and therefore forms a more efficient healing agent. The effect of complementary B and N additions on the Cu and Au precipitation kinetics has been clarified.

To couple the defect formation and healing processes, creep experiments at a temperature of 550°C were performed both at constant stress and at constant strain rate for Fe-Au alloys [6]. The influence of small amounts of Au on the nucleation and growth of creep cavities has been studied by electron microscopy. We observe that Au precipitates are formed preferential at creep cavity nucleation sites: 1) grain boundaries perpendicular to the stress direction; 2) grain boundary triple points. This site-specific Au precipitation at defect sites is found to significantly extend the creep life time of the alloy. Our results on Fe-Au model alloys demonstrate that self-healing of creep damage can be achieved in Fe-based alloys.

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**Notes**

# Modeling non-equilibrium dynamics at the nanoscale: Selected challenges and perspectives

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Supercomputing Centre Jülich, Forschungszentrum Jülich, Jülich, Germany

Modeling nanometer-scale phenomena is usually achieved by representing materials in terms of atoms, which are jiggled around in simulations as a function of their interactions and their coupling to thermostats or external fields. The interactions between atoms are deduced either from force fields or from first principles, density functional theory (DFT) being today's most popular method. A common belief is that most properties of the system under consideration could be deduced if the force fields or the density functional were sufficiently accurate. However, this becomes problematic when electrons are not in global equilibrium but only locally. A prominent example is the atom-based representation of a battery. Even if DFT can, in principle, make accurate predictions for the work function of an isolated anode, it fails to predict how the voltage between anode and cathode is affected by an electrolyte separating the anode from the cathode. As a consequence, DFT cannot be used, in its present formulation, to model non-equilibrium processes, such as the discharge of a battery. Similar problems arise in force-field based simulations, even if they are based on reactive potentials allowing the description of charge-transfer. In my talk, I present first steps to tackle this problem and to model processes such as the discharge of a battery from atomistic principles. If time permits, I will also discuss a recently proposed model to connect non-equilibrium, atomic-scale simulations of switchable materials to continuum theory.

**Notes**

# **Advanced TEM methods based on correction of the chromatic aberration**

Joachim Mayer\*

Gemeinschaftslabor für Elektronenmikroskopie (GFE), RWTH Aachen

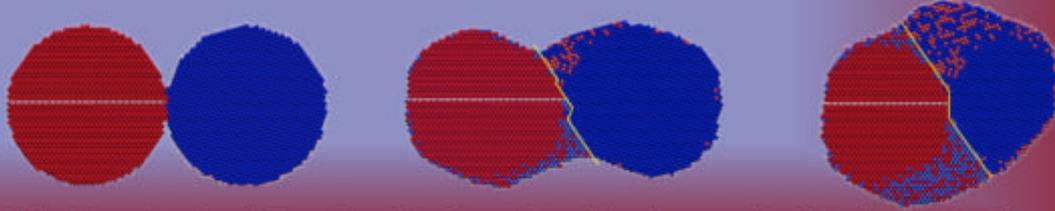
and

Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen, Forschungszentrum Jülich

**Notes**



## Poster Presentations



MiFuN – Microstructural Functionality: Dynamics, Adaption, and Self-Healing at the Nanoscale

(In alphabetical order of the first author's last name)

# Simulation of current-activated pressure-assisted densification

Sebastian Angst<sup>1\*</sup>, Gabi Schierning<sup>2</sup>, Dietrich E. Wolf<sup>1</sup>

<sup>1</sup> Department of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany

<sup>2</sup> Faculty of Engineering and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany

Cohesive particles usually form very porous agglomerates. They support loads up to a consolidation pressure, which increases with decreasing particle size. Compaction of nano-powders can therefore be very costly and time consuming. If the particles are electrically conducting, which is the case e.g. for novel nano-structured thermoelectric materials, the technique of current-activated pressure-assisted densification (CAPAD) turns out to have many advantages [1]. Electrical power deposited locally as Joule heat lowers the consolidation pressure such that higher densities without much coarsening are obtained. We present a new model combining particle dynamics, calculated by molecular dynamic methods, with a network model including thermoelectric properties [2].

[1] Z. Munir et al., *J. Mater. Sci.* **41** (2006), 763

[2] S. Angst, G. Schierning, D. E. Wolf, *AIP Conference Proceedings* **1542** (2013), 593

**Notes**

# Corrosion inhibition by galvanic integration of nanocapsules

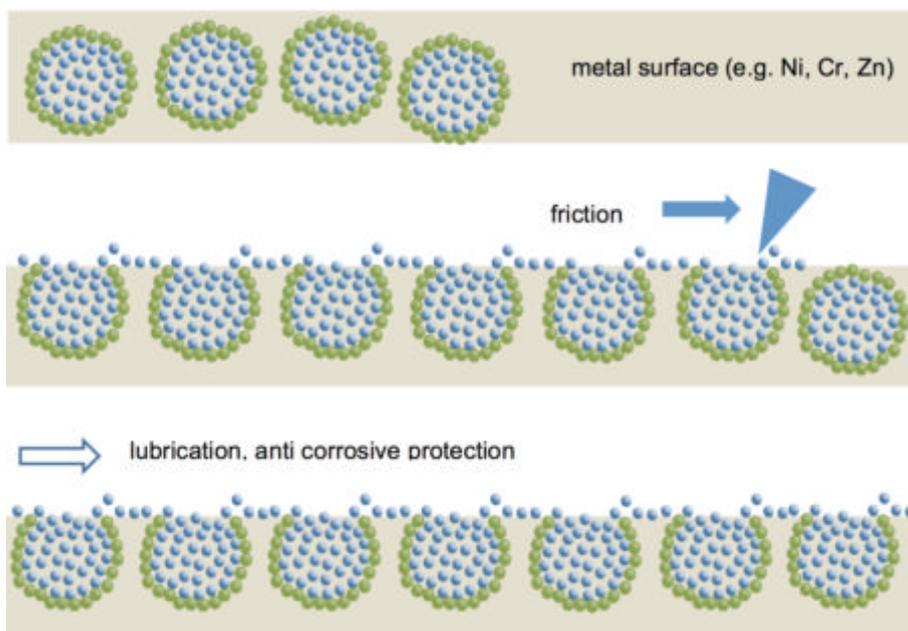
Martina Cybik\*, Christian Mayer

Physical Chemistry, University of Duisburg-Essen, Essen, Germany

Functional reagents are enclosed into polymer nanocapsules with diameters around 300 nm. These are incorporated into metallic surfaces to establish functionalities like local lubrication or corrosion protection. The integration of the nanocapsules is done by a modified Ni-Watts galvanic process. The verification of the embedding is done by AFM. The surface is analyzed in non-contact mode. AFM force-deformation experiments are used to positively identify the embedded capsules. In case of encapsulated lubrication agents, the new functionality is proven by tribological analysis.

Due to the fact that the standard polycyanoacrylate nanocapsules show a negative zeta potential, the electrophoretic migration of these particles during the electroplating step initially directs to the wrong (positive) electrode. Thus positive zeta potentials which can be achieved by cationic polymers (e.g. Chitosan) are required.

In the final product, the active ingredient is released by a local friction, hereby initiating functions such as lubrication and surface protection (Fig. 1).



**Fig. 1:** Process of friction and the resulting release of active component.

**Notes**

# Self-healing effect of functionalized surfaces

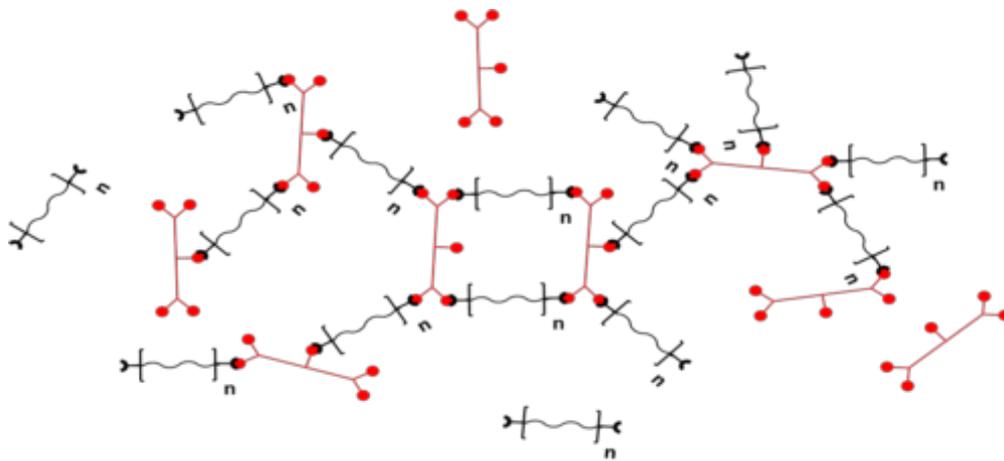
Martina Cybik\*, Nils Zelinski, Christian Mayer

Physical Chemistry, University of Duisburg-Essen, Essen, Germany

Functional reagents are enclosed into polymer nanocapsules with diameters around 300 nm. These are incorporated into paint surfaces to establish self-healing functionalities.

Epoxy resin and Diethylenediamine are encapsulated separately. Both kinds of nanocapsules are embedded in a paint layer. Nanocapsules are opened by local damage. On contact between the Epoxy resin and the Diethylenediamine a polymer resin is formed (Fig. 1) [1]. Because the scratches are now partially filled with resin, crack propagation is stopped.

[1] N. Zelinski, Synthese und Einkapselung von Reaktivharzkomponenten für selbstheilende Oberflächen, Bachelorarbeit (2014)



**Fig. 1:** Schematic presentation of the polymerisation reaction of Diethylenediamine and Epoxy resin

**Notes**

# Numerical analysis of microlattices: Ultralight, quite tight, and smart by adaption with memory

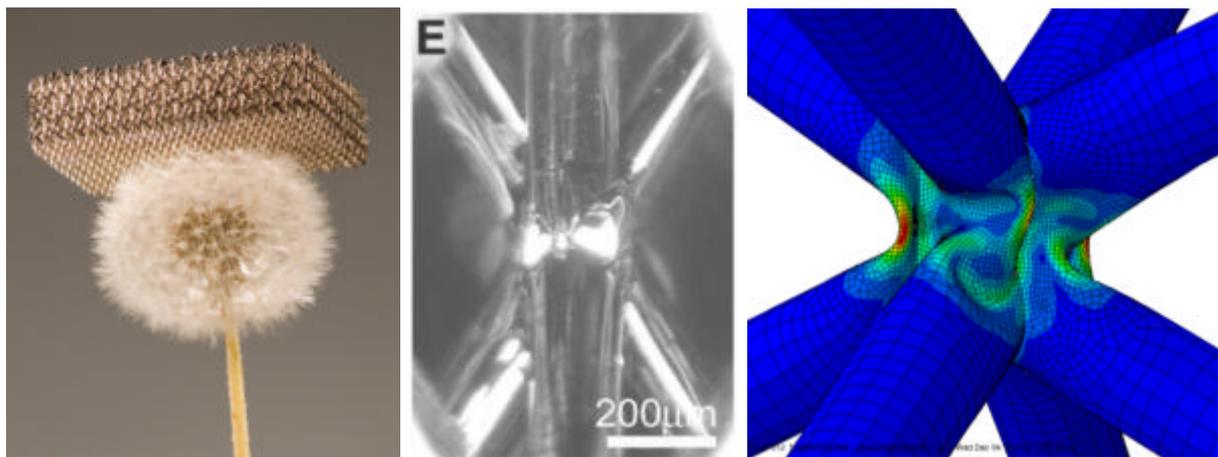
Bernhard Eidel\*

Institute of Mechanics, Faculty of Engineering, University of Duisburg-Essen, Essen, Germany  
Chair of Computational Mechanics, University of Siegen, Siegen, Germany

Microlattices as a regular, non-stochastic composition of thin-walled cylindrical shell structures have been arising considerable interest both in academia and industry in very recent years due to their exceptional mechanical properties; they are not only ultralight with a specific weight of 1% of styrofoam, (left of Fig. 1). Moreover, they exhibit singular deformation characteristics such as almost fully elastic recovery after unloading even for compressions up to 50%, [1, 2], which are favorable and in sharp contrast to stochastic open cell foams.

The objective of the present work is the modeling of microlattices and the identification of the key driving mechanisms which induce the exceptional deformation characteristics. Our finite element analysis indicates that the microlattice adapts to external loadings in terms of a local stiffness reduction by means of buckling microstructures, (centre and right of Fig. 1). This process makes the material smart since it allows for large deformations that are almost purely elastic, hence reversible. Since suchlike adaption takes place in the (i) first loading cycle (compression and unloading) beyond a threshold loading and (ii) persists for the lifetime of the lattice, it can be understood as (i) the learning phase of structural adaption that is (ii) endowed with memory. Our simulations reveal that, remarkably, the key mechanism of adaption is local buckling following from structural instability, which is a typical failure mode of standard, thin-walled structures. Here, however, buckling reduces stiffnesses on purpose and thereby enables a smooth, almost fully reversible large deformation kinematics of the microlattice.

- [1] T. A. Schaedler, A.J. Jacobsen, A. Torrents, A. E. Sorensen, J. Lian, J. R. Greer, L. Valdevit, and W. B. Carter, *Science* **334** (2011) 962.
- [2] A. Torrents, T. A. Schaedler, A. J. Jacobsen, W. B. Carter, and L. Valdevit, *Acta Mater.* **60** (2012), 3511.
- [3] <http://www.cnet.com/news/breakthrough-material-is-barely-more-than-air/>
- [4] B. Eidel, in preparation (2014).



**Fig. 1:** Microlattice supported by a dandelion seed head (left), from [3]. Buckling modes at the nodal intersections of the hollow, cylindrical struts for shell thickness  $t = 150$  nm (centre) in the experiment from [1] and (right) from finite element analysis [4] in agreement with the experiment.

**Notes**

# Phase segregation in Fe based bimetallic nanoparticles

Anna Elsukova\*, Marina Spasova, Zi-An Li, Mehmet Acet, Michael Farle

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We report on the formation of metastable alloy phases of immiscible binary systems and their transformation after thermal treatment in Fe-Cu and Ag-Fe gas-phase nanoparticles. The particles are prepared by DC magnetron sputtering. The experimental setup incorporates the furnace so the particles may be annealed during their flight prior to deposition on a substrate. The structure and morphology of the particles were investigated by High-Resolution Transmission Electron Microscopy (HRTEM). The elemental concentration and distribution was studied by means of Electron Dispersive X-ray (EDX) spectroscopy and Energy Filtered TEM.

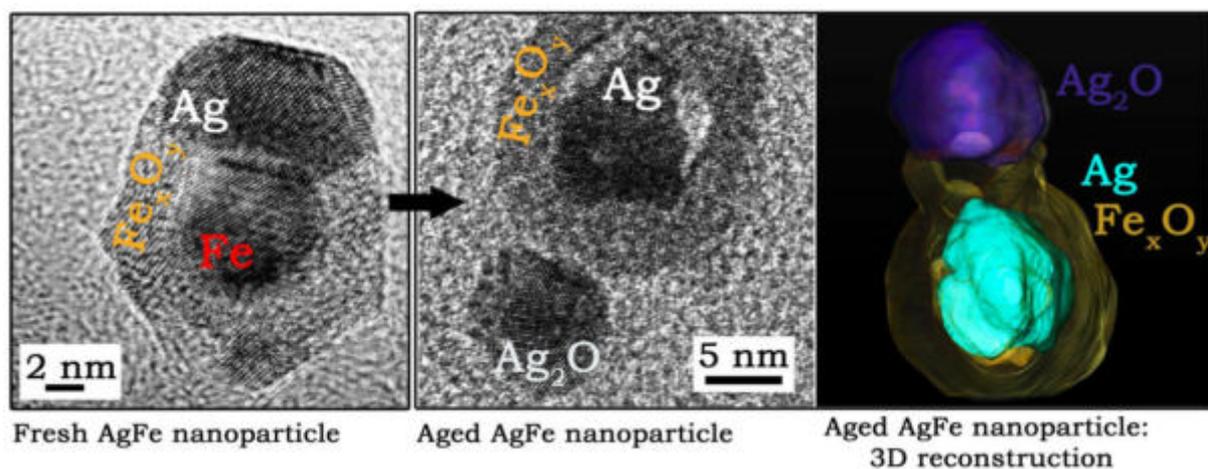
$\text{Fe}_{75}\text{Cu}_{25}$ ,  $\text{Fe}_{60}\text{Cu}_{40}$  and  $\text{Fe}_{25}\text{Cu}_{75}$  nanoparticles were obtained at 1 mbar pressure without annealing (primary) and after being in-flight annealed at  $1000^\circ\text{C}$ . Due to the fast cooling rate during sputtering metastable Fe-Cu alloy phase is fixed in as-prepared particles. Annealing leads to a phase separation via spinodal decomposition.

Two types of Ag-Fe nanoparticles with Janus (dumbbell and 'raspberry') [1] morphologies were produced at 0.5 mbar pressure after in-flight annealing at  $1000^\circ\text{C}$ . Both dumbbell and 'raspberry' particles aged over time under atmospheric conditions. As a result of the ageing of dumbbell Ag-Fe particles, part of the faceted Ag piece evolves into a spherical  $\text{Ag}_2\text{O}$  particle which in some cases is separated entirely from the rest of the composite. The  $\text{Fe}@Fe_x\text{O}_y$  part oxidizes completely into a hollow oxide shell particle and encapsulates the rest of the silver inside (see Fig. 1). The 'raspberry' particles age in a similar fashion, only silver is fully encapsulated by iron oxide shell [2].

Financial support by the DFG, SFB 445 is acknowledged

[1] A. Perro, et al., *J. Mater. Chem.* **15**, 3745 (2005).

[2] A. Elsukova et al., Structure, morphology, and aging of Ag-Fe dumbbell nanoparticles, *Phys. Status Solidi A* **208**, 2437 (2011)



**Fig. 1:** HR-TEM images of the structure and chemical composition of dumbbell a Ag-Fe nanoparticle before and after ageing

**Notes**

# A conceptual study into the potential of MAX-Phase Ceramics for self-healing of crack damage

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<sup>1</sup> Department of Materials Science and Engineering, Delft University of Technology, Delft, The Netherlands

<sup>2</sup> Faculty of Aerospace Engineering, Delft University of Technology, Delft, The Netherlands

The reduction of maintenance and replacement work costs is an important driving force in the development of high temperature materials ( $T > 800^{\circ}\text{C}$ ) that can autonomously heal damage as a result of local cracks. In recent years some potential routes involving the addition of sacrificial particles have been identified, yet these systems have the drawback of reduced initial properties and being capable of healing cracks only once. Hence there is a need for high temperature materials with high initial properties and an ability to heal cracks several times.

$\text{Ti}_2\text{AlC}$ , being a member of the MAX-Phase ceramics family has shown an unusual ability to heal cracks multiple times through selective oxidation of Al, while maintaining its salient mechanical properties [1]. It is to be expected that other compounds of the  $\text{M}_{n+1}\text{AX}_n$  family, where M is a transition metal, A an element from groups 13 or 14 and X either Carbon or Nitrogen combining characteristics of metals and ceramics, may also show (as yet unidentified) self-healing abilities.

In this work all MAX phases known to date (approx. 70) have been evaluated to establish a group of potential compounds expected to be promising applicants of (multiple) crack-healing. To this end, their thermodynamics and material transport at elevated temperatures determining the selective oxidation kinetics and crack filling potential have been considered.

MAX phases with Al and Si are of special interest since the oxides of these A elements have been shown to act successfully as healing agents [2, 3]. While not having been explored, MAX phases which in combination with the oxidation of the M element form a single ternary oxide may also offer attractive self-healing potential.

MAX phases that show an above average potential for self-healing have been identified, in order to guide the experimental research into the wider exploration of MAX phase ceramics for intrinsic high temperature self-healing ceramics.

Financial support by the People Programme (Marie Curie ITN) of the European Union's seventh framework programme, FP7, grant number 290308 (SHeMat) is acknowledged.

- [1] Li, S., et al., Multiple crack healing of a  $\text{Ti}_2\text{AlC}$  ceramic. *J. Eur. Ceram. Soc.*, **2012**. 32(8): p. 1813-1820.
- [2] Yang, H.J., et al., High temperature healing of  $\text{Ti}_2\text{AlC}$ : On the origin of inhomogeneous oxide scale. *Scripta Mater.*, 2011. **65**(2): p. 135-138.
- [3] Osada, T., et al., Strength recovery behavior of machined  $\text{Al}_2\text{O}_3/\text{SiC}$  nano-composite ceramics by crack-healing. *J. Eur. Ceram. Soc.*, 2007. **27**(10): p. 3261-3267.

## Notes

# Constructive electromigration of indium on silicon (111)

P. Graf, A. M. Bernhart, M. R. Kaspers, C. A. Bobisch\*, and R. Möller

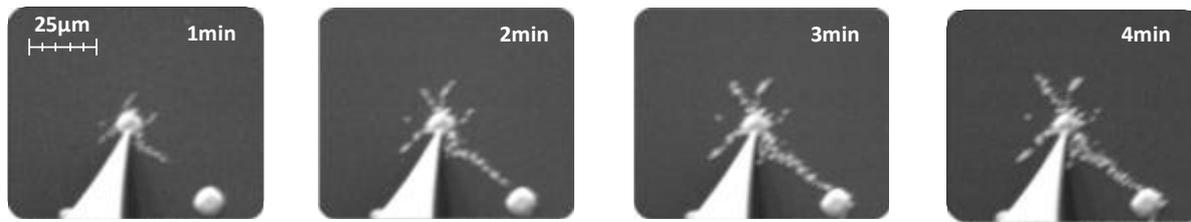
Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany

Electromigration (EM) is the material transport driven by an electron current or by an electric field [1]. This process is technically very important for thin/small conductors in electronic devices (e.g. CPUs) since the dimension of such structures reach the range of 10 nm or less. Here, we investigate in situ the EM of Indium on a Si (111) surface using a four probe scanning tunneling microscope (STM) and a scanning electron microscope (SEM). We study the indium induced surface reconstruction on Si (111) [2] with  $\mu\text{m}$ -scaled indium islands. To apply an electric field in parallel to the surface two tips make contact to islands. Using the SEM we observe the formation of additional In islands in between the contacted islands, which results from the material transport from the indium reconstruction.

In contrast to the usual destructive EM, we use this transport to form Indium wires. The method may become a starting point for the directed growth of small electronic networks.

[1] R. Landauer and W. Woo, *Phys. Rev. B* **10**, p. 1266 (1974).

[2] Eli Rotenberg et al., *Phys. Rev. Lett.* **91**, 246404 (2003).



**Fig. 1:** Electromigration of Indium on Si (111) during 4 minutes at the negative pole. The transverse current is about 5 mA.

**Notes**

# Inkjet printing and laser sintering of metal oxide nanoparticles

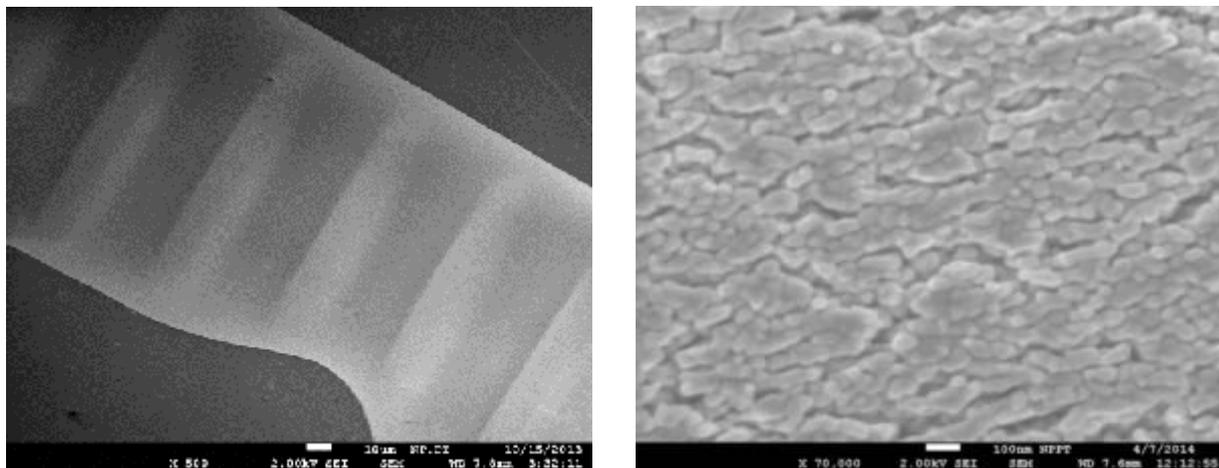
Lukas Helmbrecht\*, Julia Susanne Gebauer, Christian Notthoff, Gerd Bacher and Markus Winterer

Nanoparticle Process Technology, Faculty of Engineering and CENIDE, University of Duisburg-Essen, Duisburg, Germany

Inkjet printing of nanoparticles for the fabrication of devices such as transistors, biomaterials, sensors, photo catalysts, solar cells or 3D-objects has gained much attention in the last decade [1-4]. Depending on the application, homogeneous and dense films are desired, which can be realized by laser sintering of the printed material. Laser sintering is advantageous over other thermal treatments, due to much shorter processing time, efficient energy deposition and localized heat load which makes it ideal for printing on flexible substrates [5].

Due to their wide band gap, printed semiconductor structures from materials like ZnO and TiO<sub>2</sub> are of great interest for the industry. Besides this the functional properties and lifetime of the printed structures depend mainly on their crystallinity and homogeneity. In this work the formation of printed metal oxide structures from chemical vapor synthesized ZnO and TiO<sub>2</sub> nanoparticles was studied with SEM and profilometry. Furthermore insights on structural changes resulting from laser post processing through simulation, XRD and photoluminescence spectroscopic measurements are given.

- [1] R. F. Pereira, C. C. Barrias, P. L. Granja, and P. J. Bartolo, *Nanomed.* **8** (2013) 603-621
- [2] S. Dasgupta, R. Kruk, N. Mechau and H. Hahn, *ACS nano* **5** (2011) 9628-9638
- [3] K. Sun, T.-S. Wei, B. Y. Ahn, J. Y. Seo, S. J. Dillon and J. A. Lewis, *Adv. Mater.* **25** (2013) 4539-4543
- [4] A. S. Khalil, S. Hartner, M. Ali, A. Gupta, H. Wiggers, and M. Winterer, *J. Nanosci. Nanotechn.* **11** (2011), 10839-10843
- [5] A. Sandmann, C. Notthoff, and M. Winterer, *J. Appl. Phys.* **113** (2013) 0044310.



**Fig. 1:** SEM images of an inkjet printed and laser sintered TiO<sub>2</sub>-structure. (left) The laser-sintering-paths derived from the use of a focused continuous wave HeCd-laser (325 nm) are clearly visible on the printed structure. (right) HR-SEM image of the sintered TiO<sub>2</sub>-nanoparticles.

**Notes**

# GaN/GaN nanowire-based LEDs on silicon (111)

R. Koester, Christian Blumberg, G. Keller, W. Prost\*, F.-J. Tegude, Daniel Sager, and Gerd Bacher

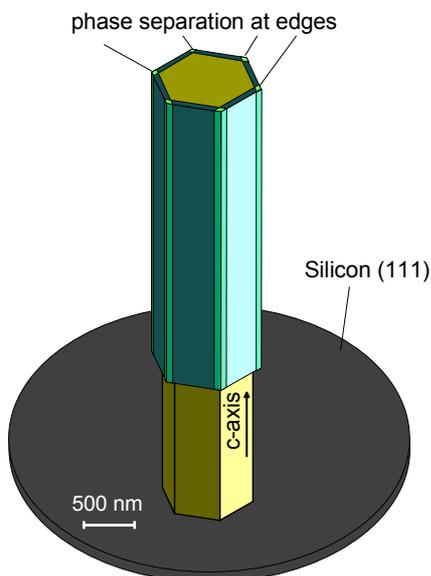
University Duisburg-Essen, Faculty of Engineering, Institute of Information Technology, Duisburg, Germany

GaN and related III-nitrides are nowadays the material of choice for the fabrication of bright light emitting devices (LEDs) which are used for illumination, traffic lights and for background illuminated LCD displays. In the recent years GaN nanowires (NWs) gained more and more attention as building blocks for one dimensional GaN structures [1, 2]. Recently, a GaN NW based InGaN/GaN multi quantum well (MQW) LED structure has been developed on insulating sapphire by a self-assembled MOVPE approach [3]. The commonly used c-plane growth results in strong internal electrical fields due to spontaneous polarization, causing long carrier life-times and hence low LED operation speed. This issue can be overcome by the access to the NWs m-plane side facets, which are usually free from strong internal electrical fields, enabling the fabrication of high speed LEDs suitable for optical communication.

In this work we present the NW growth and electroluminescence results of an m-plane core-shell p-i-n InGaN/GaN quantum well structure on n-GaN NWs grown on conductive n-Silicon (111) substrates. The substrate conditioning procedure as well as the AlN buffer layer deposition is crucial for the formation of vertical growing GaN NWs on the Si (111) surface. Due to the demand of silane during the growth, the NWs exhibit strong n-type doping. The as grown NWs can be used as templates for the growth of GaN NW based InGaN/GaN MQW LED core-shell structures. By changing the growth parameters to the conventional 2-D layer growth conditions an InGaN/GaN MQW and p-GaN layer is deposited as a shell growing in m-plane direction around the n-doped NWs. The vertical standing NW based LED array is electrically contacted by metallic contacts for I/V- and electroluminescent characterization. The LED exhibits electro-luminescence visible to the naked eye at a forward bias voltage around 4 V. The bandwidth of emission after short electrical pulse excitation exceeds 1 GHz (Fig. 1). Further works focus on the combination of high speed emission and larger wavelength in the green and in the red. For this purpose the fabrication of InGaN quantum dots on the m-plane facets are aimed at. While nanowires of a high degree of lattice mismatch accommodation along the growth direction exploited here for GaN growth on Si, the lattice constants are fixed on facets enabling QD formation along the edges and on the facets.

## References

- [1] A. Kikuchi et al., *Jap. J. Appl. Phys.* **43**, No. 12A, pp. L1524-L1526, 2004
- [2] S. D. Hersee et al., *IEEE Electronics Letters* **45**(1), 2009.
- [3] R. Koester et al., *Nano Letters* **11**, 4839–4845, 2011.



**Fig.1:** Sketch of a InGaN /GaN nanowire LED with phase separation at the edges aiming at high-speed long wavelength emission

**Notes**

# Silver doping of Cadmium selenide – function and structure

Alexander Kompch<sup>1\*</sup>, Ayaskanta Sahu<sup>2</sup>, Christian Notthoff<sup>1</sup>, Florian Ott<sup>3</sup>, David J. Norris<sup>3</sup> and Markus Winterer<sup>1</sup>

<sup>1</sup> Nanoparticle Process Technology, Faculty of Engineering and CENIDE, University of Duisburg-Essen, Duisburg, Germany

<sup>2</sup> Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, USA

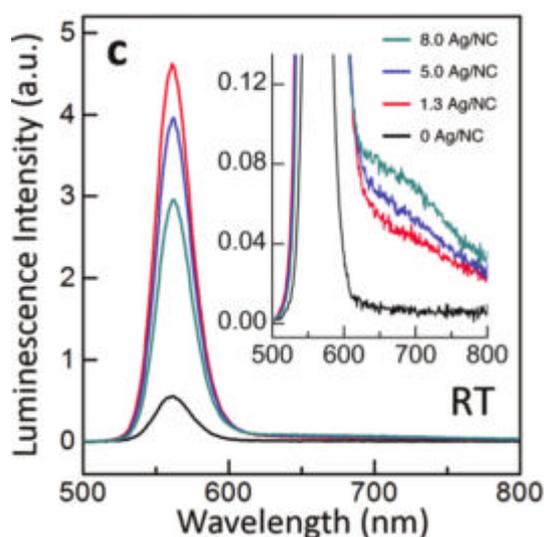
<sup>3</sup> Optical Materials Engineering Laboratory, ETH Zurich, Zurich, Switzerland

Cadmium selenide (CdSe) nanocrystals are doped with Silver (Ag) impurities and their optical and structural properties are investigated. Even though CdSe is the most studied nanocrystal system, surprising changes in the fluorescence are observed upon addition of only a few Ag atoms per nanocrystal. The fluorescence is dramatically enhanced peaking at about 2 Ag atoms per nanocrystal and then slowly decreases at higher concentrations (Fig. 1). Ag would be expected to act as an acceptor substituting for Cd but this nonmonotonic trend suggests a more complex local environment of the dopant including a possible change of the Ag position inside the nanocrystal [1]. The local structure around the Ag atom is investigated by X-ray absorption spectroscopy (XAS) at the K-edges of Cd, Ag and Se. Using Reverse Monte Carlo (RMC) simulations [2], we refine all three spectra with a single, mutual configuration of atoms (Fig. 2) for various possible positions of Ag inside the nanocrystal to obtain consistent structural information [3]. We find that Ag sits on a tetrahedral interstitial site acting as a shallow donor and as a deep level defect at higher Ag content.

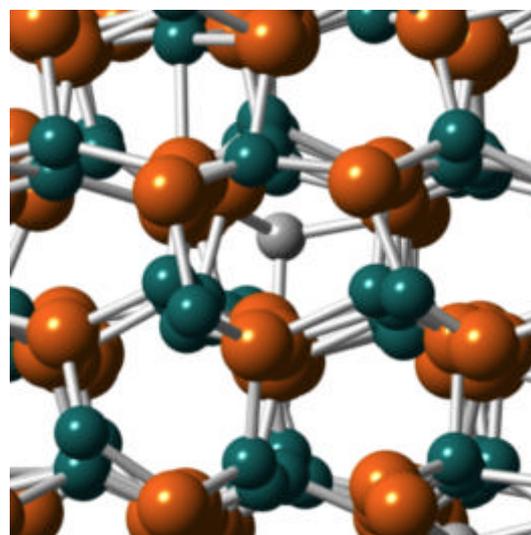
[1] A. Sahu, M. S. Kang, A. Kompch, C. Notthoff, A. W. Wills, D. Deng, M. Winterer, C. D. Frisbie and D. J. Norris, *Nano Letters*. **12** (2012), 2587

[2] M. Winterer, *J. Appl. Phys.* **88** (2000), 5635

[3] R. Djenadic, G. Akgul, K. Attenkofer and M. Winterer, *J. Phys. Chem. C* **114** (2010), 9207



**Fig. 1:** Room-temperature fluorescence spectra for 3.0-nm-diameter CdSe nanocrystals dispersed in hexanes with Ag content as indicated



**Fig. 2:** Best model obtained from RMC simulations: a cylindrical Ag-doped CdSe nanocrystal with wurtzite structure (projection along b-axis, Cd:green, Ag:silver, Se:orange)

**Notes**

# Self-learning kinetic Monte Carlo: Modeling homoepitaxial growth and electromigration induced void and island drift

Andreas Latz\*, Lothar Brendel, Simon P. Sindermann, G. Dumpich, Frank-J. Meyer zu Heringdorf, and Dietrich E. Wolf

Computational and Statistical Physics, Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany

The self-learning kinetic Monte Carlo (SLKMC) method [1] combines the calculation of transition rates from a realistic potential with the efficiency of a rate catalog, using a pattern recognition scheme. Originally limited to twodimensional systems with one specific surface orientation, we recently extended the method to three dimensions and arbitrarily shaped surfaces [2,3]. We showed that by setting up an initial database, which can be done perfectly in parallel, the concomitant huge increase of rate calculations on the fly can be decreased significantly.

The model is applied to the homoepitaxial growth of Ag on Ag (111) at low temperatures and the electromigration-induced void and island drift on unpassivated surfaces of single crystal metallic films at the atomic scale. Depending on the combination of the surface texture and the direction of the applied electric field, the void or island drift direction is not necessarily aligned anti-/parallel to the electric field direction [4].

- [1] O. Trushin et al., *Phys Rev. B* **72** (2005), 115401
- [2] A. Latz, L. Brendel, and D. E. Wolf, *J. Phys.: Condens. Matter* **24** (2012), 485005
- [3] A. Latz, L. Brendel, and D. E. Wolf, *MRS Proceedings* (2013), 1559
- [4] A. Latz et al., *J. Phys.: Condens. Matter* **26** (2014), 055005

**Notes**

# Surface reconstruction of gold nanocrystals and their coalescence under electron beam irradiation

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<sup>1</sup> Faculty of Physics and CeNIDE, University of Duisburg-Essen, Duisburg, Germany

<sup>2</sup> Centre de Recherche Paul Pascal, CNRS, Pessac, France

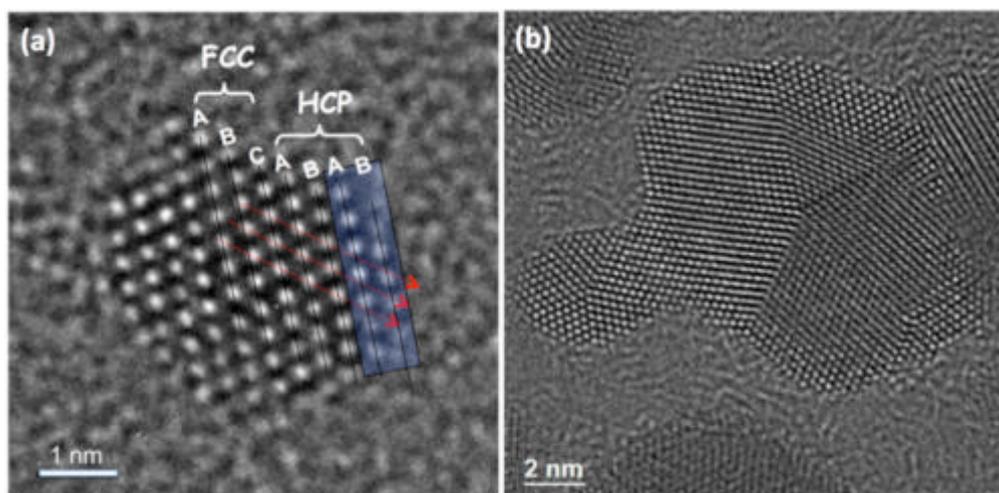
Research interest in nanoscale particulates of noble metals continuously grows across a broad range of technical and scientific disciplines [1]. Gold nanocrystals and their derived forms of thin film or granules provide additional advantages through size or surface effects and superior properties making them truly advanced materials of great importance [2]. However, detailed knowledge about their crystal structure, in particular the atomic surface structure, and the stabilities of particles under external stimuli have to be addressed for realization of their full potentials in applications.

Here, using high-resolution transmission electron microscopy (HRTEM) we present our results of the structural and compositional characterizations of colloidal-chemistry-synthesized gold nanocrystals and their ensembles, with a particular focus on the surface structure of nm-sized gold NCs and the stability of particles under strong electron irradiation. We find that for small gold NCs of 1-2 nm, its surface atoms can reconstruct into hexagonal-close-packed atomic arrangement, which is in stark contrast to the bulk with typical face-centered-cubic (FCC) structure, as shown in figure (a). With increasing sizes from 2 to 10 nm, gold nanocrystals dominantly are in the form of multiple-twinned particles, e.g., decahedral- and icosahedral-shaped, reflecting strong competitions between surface, twinning, grain boundaries and internal lattice strain energies. We note that due to the HRTEM imaging conditions when gold NCs are bombarded by 300 keV electrons their pristine structures are disturbed. Therefore, we studied the effects of electron beam irradiation on the structure stability of particles in more detail. We find that at weak ( $\sim 1 \times 10^4$  electron/nm<sup>2</sup>), moderate dose of electron irradiation, the gold NCs stay stationary on the supporting carbon film with unnoticeable motion. With increasing electron flux density ( $\sim 2 \times 10^5$  electron/nm<sup>2</sup>) and prolonged irradiation, particles of sizes (2-5 nm) become mobile (rotationally and translationally) on supporting carbon films. At higher electron flux density ( $\sim 5 \times 10^7$  electron/nm<sup>2</sup>), the particles began moves either towards or against each other. Once the particles came into contact, fast coalescence began and quickly crystallized into one bigger particle, as shown in figure (b). The detailed of the particles motion and coalescence will be presented and the underlying mechanism will be discussed.

Work was performed at ERC, FZ Jülich with the help of Dr. J. Bartel. Financial support by the EU through the programs REFreePermag and IMAGINE is acknowledged.

[1] Tao, A. R.; Habas, S.; Yang, P. *Small*, **4**, 310 (2008)

[2] Langille, M. R.; Zhang, J.; Personick, M. L.; Li, S. Y.; Mirkin, C. A. *Science*, **337**, 954 (2012)



**Fig. 1:** (a) Surface structure of gold nanocrystals with hexagonal-close packed structure at the particle surface. (b) Particles coalescence under 300 keV electron beam irradiation.

**Notes**

# Trapping of photophoretic particles

Martin P. Magiera\*, Lothar Brendel

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In the last decade various approaches have been pursued to construct artificial active swimmers and to understand their collective behavior. These nano- and micron-sized objects are fascinating due to their intrinsic out-of-equilibrium nature and the fact that they swim at low Reynolds numbers. Possible applications in drug-delivery, lab-on-the-chip devices or self-assembly are other driving forces for the increasing research in this field.

Several propulsion mechanisms are based on phoretic forces [1,2]. One example is self-diffusiophoresis of Janus-particles, where a concentration gradient of the solvent is created via a catalytic reaction at the particles' surface [3,4]. Another method is based on the inhomogeneous heating of Janus particles using inhomogeneous coating and laser-light [5]. This photophoretic concept does not depend on the solvent and is therefore called 'fuel-free'.

The realization of steering and trapping of artificial microswimmers is of fundamental interest. Different approaches have been addressed recently, most based on the introduction of walls [6]. Some approaches use phoretic forces [7] or complicated feedback-control mechanisms [8]. Using theory and computer simulations we show that photophoretically driven self-propelled particles can be trapped using an inhomogeneous illumination of the system setup. As this method does not imply the introduction of permanent obstacles, it is relevant for in-vivo applications and those where only a temporal trapping is required. It is not restricted to photophoretic swimmers, but can be used in several low-Reynolds-numbers-systems where the propulsion of swimmers can be switched off locally.

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**Notes**

# $\mu$ GIWAXS and electrical conductivity measurements on laser sintered metal oxide nanoparticles

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Currently, there is a great demand for low-cost fabrication methods for various electronic and optoelectronic devices, based on thin film technologies. Ink-jet printing of dispersed nano-powders is advantageous compared to other deposition techniques as it can precisely deposit small volumes of dispersions (inks) in a well defined pattern [1,2]. Metal oxide nano-powders like ZnO or TiO<sub>2</sub> are of special interest, because of their outstanding optical, electrical and thermal properties. For most applications a sintered film is desired and laser sintering is a promising technique. Compared to other methods like thermal sintering in a furnace it has the advantage that the processing time is short and the heat load is localized and controlled. The optical, electrical and thermal properties of the metal oxide nano-powders are closely related to structural characteristics and physical properties like phase composition, defect density, micro strain and crystallite size. For example the photocatalytic activity of TiO<sub>2</sub> is directly related to the phase present [3]. Recently, we have shown that the use of continuous UV lasers allows sintering of TiO<sub>2</sub> and ZnO nano-powder films with power densities down to 38 kW/cm<sup>2</sup> and a precise control of the powder bed density tuned through the applied laser power [4].

In this contribution we will present our first  $\mu$ GIWAXS measurements performed at the P03 beamline (HASYLAB) on laser sintered ZnO and TiO<sub>2</sub> nano-powder films and the influence of laser sintering on the electrical properties of ZnO. Furthermore, we describe the laser heating process numerically using an iterative finite element algorithm, which couples the heat equation with a simplified sintering model. The numerical and experimental results match well and reveal two key parameters responsible for the effective heating and sintering process: The laser wavelength in relation to the band gap of the material and the initial porosity of the film.

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**Notes**

# Chemical vapor synthesis of nanocrystalline ZnFe<sub>2</sub>O<sub>4</sub> powder and its sintering

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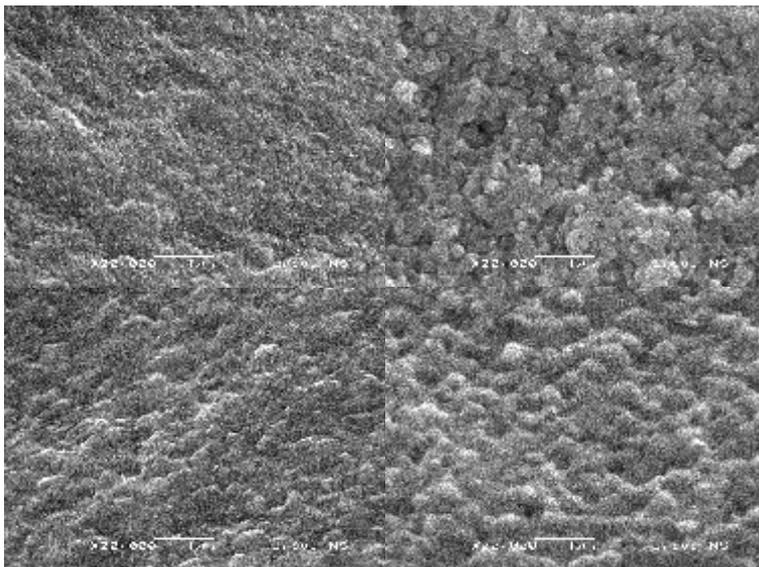
<sup>1</sup> Nanoparticle Process Technology, Institute for Combustion and Gas Dynamics, and CENIDE, University of Duisburg-Essen, Duisburg, Germany

<sup>2</sup> Department of Materials Engineering, Faculty of Technology, University of Novi Sad, Serbia

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For microwave applications, in addition to high electrical resistivity, high density is required for good magnetic permeability, flux density and susceptibility. Powders synthesized by the chemical vapor synthesis (CVS) are known to have good sinterability [1] and are thus good candidates for production of spinel ferrites for microwave devices. ZnFe<sub>2</sub>O<sub>4</sub> powders were synthesized by the CVS method and their nanocrystalline structure was confirmed by XRD and TEM. The powders were subsequently uniaxially pressed into pellets and sintered at 800, 900 and 1000°C. Fresh fracture surface of the green and sintered pellets were examined by SEM.

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**Fig. 1:** SEM images of the fresh fracture of ZnFe<sub>2</sub>O<sub>4</sub> pellets pressed and sintered at different temperatures

**Notes**

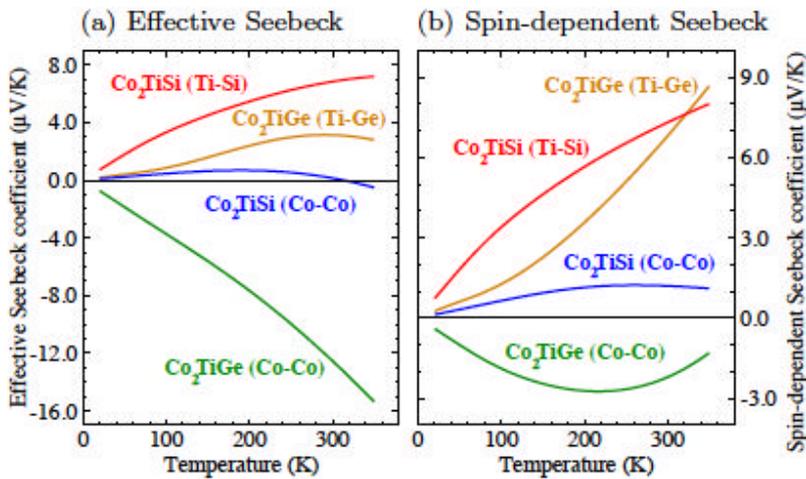
# Interplay of growth mode and thermally induced spin accumulation in epitaxial Al/Heusler alloys contacts

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Spin injection from a ferromagnet in a semiconductor substrate can be accomplished either by applying an external voltage or a temperature gradient. In the latter case, one exploits the Seebeck effect, with the temperature gradient across the contact directly resulting in a difference in chemical potentials in the two spin channels due to the spin-dependence of the Seebeck coefficient. The magnetic Heusler alloys  $\text{Co}_2\text{TiSi}$  or  $\text{Co}_2\text{TiGe}$  exhibit half-metallic ferromagnetism in their ideal L21 crystal structure, with a potentially high degree of spin polarization of the injected current. As such, they recommend themselves for integrated spin injectors in combination with the closely lattice-matched Al contact layer.

We investigate the possibility of employing Al/ $\text{Co}_2\text{TiX}$ /Al ( $X=\text{Si,Ge}$ ) trilayers as thermally driven spin injectors by means of first-principles calculations of the electronic structure and of the thermoelectric transport properties. Our results show that the spin-dependent Seebeck effect is sensitive to the atomic structure of the Heusler/Al interface. In particular, for a thin  $\text{Co}_2\text{TiSi}$  or  $\text{Co}_2\text{TiGe}$  layer terminated by a TiSi or TiGe atomic plane, the thermal spin accumulation is found to be of the same order of magnitude as the effective Seebeck coefficient.



**Fig. 1:** (a) Effective and (b) spin-dependent Seebeck coefficients for the Al/ $\text{Co}_2\text{TiSi}$ /Al and Al/ $\text{Co}_2\text{TiGe}$ /Al trilayer systems as a function of temperature and interface termination (Co-Co or Ti-Z).

**Notes**

# Modeling of Au-catalyzed GaAs nanowire growth

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The semiconductor nanowires in focus of our research are spontaneously evolving structures, e.g. in molecular beam epitaxy, due to large anisotropies in growth speed. In addition, a metal catalyst particle (e.g. a gold particle of ~50 nm in diameter) may be used as a promoter, e.g. to fabricate a GaAs nanowire that grows perpendicularly out of the Au-GaAs interface. While the driving force for growth is the chemical non-equilibrium between the gas phase, the liquid Au-alloy particle and the solid GaAs wire, the geometrical shape of the nanowire and catalyst particle are determined by the mechanical equilibrium at the boundary between these phases.

In order to gain theoretical insight into nanowire growth, we combine an atomistic description of the energetics with concepts from macroscopic thermodynamics and kinetics. Using judiciously chosen periodic supercells, density functional theory (DFT) calculations provide us with the surface energies of the catalyst particle and the nanowire facets, as well the energy of the interface between the nanowire tip and the catalyst. This puts us in position to calculate the contact angle of wetting and the thermodynamically determined 'neck' radius of the nanowire that grows out of a catalyst particle of given volume. [1]

Moreover, DFT calculations help us to understand the role of the Au catalyst surface for the adsorption and retention of the gas-phase species [2], and to determine the potential energy surfaces (PESs) for diffusion of Ga and As adatoms and GaAs molecules adsorbed on the nanowire side facets. [3] From the energy minima and the saddle points of the PESs the energy barriers governing the diffusion process can be extracted. Ga diffusion barriers are found to generally lower than As diffusion barriers.

In summary, our calculations suggest a growth mechanism where the uptake of As<sub>2</sub> from the gas phase proceeds by dissociative adsorption on the Au surface, while Ga atoms adsorb both on the Au particle and the nanowire sidewalls. In the latter case, their fast diffusion towards the catalyst particle results in a denuded zone just below the nanowire tip, suppressing nucleation of new atomic layers on the sidewalls. Analyzing the complex interplay of adsorption, diffusion and reaction processes allows us to rationalize why the speed for axial growth can be made much higher than the radial growth speed for appropriately chosen conditions, i.e., temperature and V-III ratio in the gas phase.

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## Notes

# Synthesis and control of Silver nanowire dimensions using scavenger-mediated polyol synthesis for transparent conductive electrodes

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One-dimensional (1D) metallic nanowires have been a focus of research in the past decade due to their special physical and anisotropic properties at the nano scale [1,2]. This opens the door to a wide range of applications such as biological sensors [3] and electronic devices [4]. Silver nanowires (Ag NWs) are of special interest as bulk silver has the highest electrical and thermal conductivities of all metals [5]. Therefore, they hold big promise to be flexibly integrated in electronic devices in form of transparent conductive electrodes based on Ag NW networks.

By using the scavenger mediated polyol technique [6], Ag NWs can be synthesized and can directly be integrated in transparent conductive electrodes. This technique is simple, reproducible and robust. Therefore, an extensive parametric study was done on the synthesis conditions for Ag NW including temperature and time, precursor concentration and reaction scaling aiming at preferably long wires (several  $\mu\text{m}$ ) which permit highest conductivities (percolation threshold achieved). In addition to that, an extension of this technique was also used termed the Successive Multi-step Growth technique (SMG) [7] that has the capacity to realize even longer nanowires (50 - 200  $\mu\text{m}$ ) (Fig.1). This helps to achieve an increasingly good connecting nanowire network with high conductivity at lower surface coverage thereby increasing electrode transparency [8]. The synthesized nanowires were spin coated and spray coated and the conditions for coating were screened to find optimized electrodes that hold minimum sheet resistances and maximum transparencies. These Ag NW electrodes can be used for thin film solar cell contacts and touch panel applications as a promising candidate to replace the indium-tin oxide (ITO) layer that suffers from Indium scarcity.

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**Notes**

# Growth of (001)-textured L<sub>10</sub> FePtCu thin films on SiO<sub>2</sub> by pulsed laser deposition and rapid thermal annealing

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Chemically ordered (L<sub>10</sub>) FePt is a candidate for ultrahigh density magnetic recording media, magnetic sensors or permanent magnets due to its huge magnetocrystalline anisotropy energy density (MAE) ( $7 \times 10^6 \text{ J/m}^3$ ) [1,2]. The origin of the MAE is a tetragonal distortion along the c-direction of the L<sub>10</sub> phase, in which the easy axis of magnetization is oriented. For thin film applications, it is most favorable having an out-of-plane magnetization [3]. Thus, strongly textured films are desired with the c-axis oriented perpendicular to the film plane.

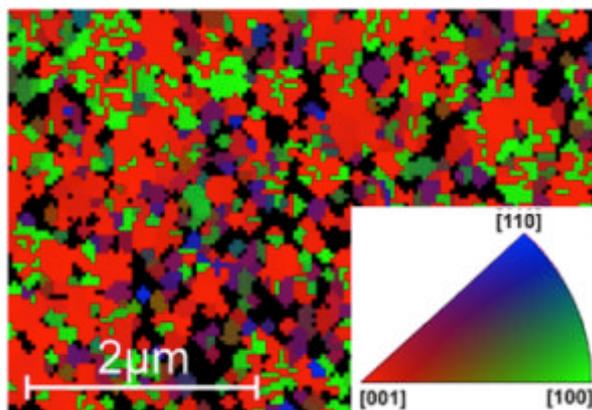
FePt thin films deposited on amorphous SiO<sub>2</sub> substrates at ambient temperature form a disordered A1 phase. To transfer the film into the L<sub>10</sub> phase subsequent annealing is mandatory. Rapid thermal processing (RTP) enables this transformation and enhances growth of (001)-oriented grains perpendicular to the film plane due to internal stress [4,5]. Additionally, Cu is known to improve diffusion while favoring the (001)-textured growth [1].

We prepared thin nanocrystalline (Fe<sub>1-x</sub>Cu<sub>x</sub>)Pt films using pulsed laser deposition (PLD). Crystal structure, morphology and magnetic properties have been studied as function of annealing temperature and time as well as Cu concentration (0 at-% up to 35 at-%). In more detail, we studied the A1-L<sub>10</sub> phase transition for annealing on the timescale of some 10 s.

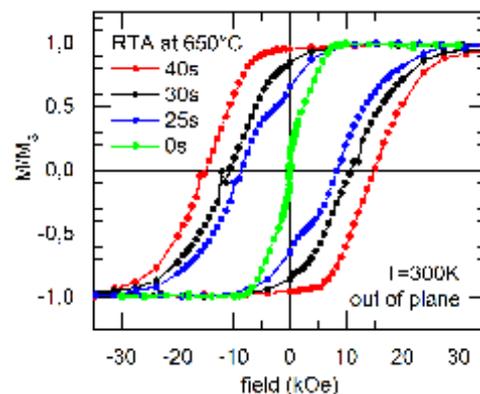
Atomic force microscopy suggests that the film surface morphology flattens with increasing Cu concentration. The RTP studies show a closed, smooth film with (001)-texture after annealing at 650°C for 30s. Figure 1 presents an electron backscatter diffraction (EBSD) micrograph showing the dominant (001) grain orientation in the film. Furthermore, the Cu content and the RTP can be used to tailor magnetic properties like HC, MS and orientation of the easy axis. Figure 2 displays out-of-plane hysteresis loops at ambient temperature after RTP at 650°C and different RTP times [5].

This project has partly been supported by the Baden-Württemberg-Stiftung.

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**Fig. 1:** EBSD analysis of a 10nm thick (Fe<sub>90</sub>Cu<sub>10</sub>)<sub>52</sub>Pt<sub>48</sub> film after RTP at T = 650°C for 30 s. The color code shows the grain orientation perpendicular to the film plane.



**Fig. 2:** Out-of-plane magnetic hysteresis loops of 10 nm (Fe<sub>90</sub>Cu<sub>10</sub>)<sub>52</sub>Pt<sub>48</sub> alloy films at 300 K for increasing RTP annealing times from 0s to 40s.

**Notes**

# Tuning the electric polarization in multiferroic $\text{CoFe}_2\text{O}_4$ / $\text{BaTiO}_3$ nanocomposites by magnetic fields

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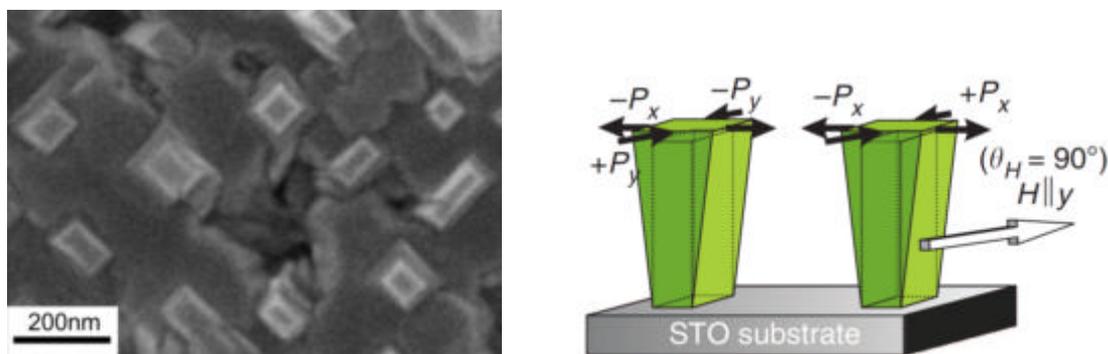
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<sup>4</sup> Department of Inorganic Chemistry and Catalysis, Universiteit Utrecht, Utrecht, The Netherlands.

Multiferroic materials showing both magnetic and electric ordering allow an additional degree of freedom in the design of actuators, transducers and storage devices and thus have attracted scientific interest from the technological perspective as well as from basic research. Because the choice of single-phase multiferroic materials being suitable at room temperature is limited, the use of magnetoelectric two-phase composites has proven to be more promising [1]. Here we study ferrimagnetic  $\text{CoFe}_2\text{O}_4$  (CFO) nanopillars embedded in a ferroelectric  $\text{BaTiO}_3$  (BTO) matrix (Fig. 1, left)). They operate at room temperature and are free of any resource-critical rare-earth element, which makes them interesting for potential applications. Prior studies succeeded in showing strain-mediated coupling between the two subsystems. In particular, the electric properties can be tuned by magnetic fields and the magnetic properties by electric fields. Here we take the analysis of the coupling to a new level utilizing soft X-ray absorption spectroscopy and its associated linear dichroism [2]. We demonstrate that an in-plane magnetic field breaks the tetragonal symmetry of the (1,3)-type  $\text{CoFe}_2\text{O}_4/\text{BaTiO}_3$  structures (Fig. 1, right)) and discuss it in terms of off-diagonal magnetostrictive-piezoelectric coupling. This coupling creates staggered in-plane components of the electric polarization, which are stable even at magnetic remanence due to hysteretic behaviour of structural changes in the  $\text{BaTiO}_3$  matrix. The competing mechanisms of clamping and relaxation effects are discussed in detail. The effect in the electric in-plane polarization of BTO obtained in this work extends over a large area. Under the constraint of completely regular arrays of CFO nanopillars, one might even envisage data-storage concepts by encoding the local polarization patterns of single nanopillars via external current-controlled local magnetic fields.

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**Fig. 1:** Left: Scanning electron microscopy image of the sample corresponding to a top view on the nanopillar structure. Right: Schematic presentation of the strained CFO nanopillars in the BTO matrix (not shown) when applying a magnetic field perpendicular to the pillars [2].

**Notes**

# Interaction of electromigration driven voids and the crystal lattices of bi-crystalline Ag-nanostructures

Simon P. Sindermann\*, Günter Dumpich, and Frank-J. Meyer zu Heringdorf

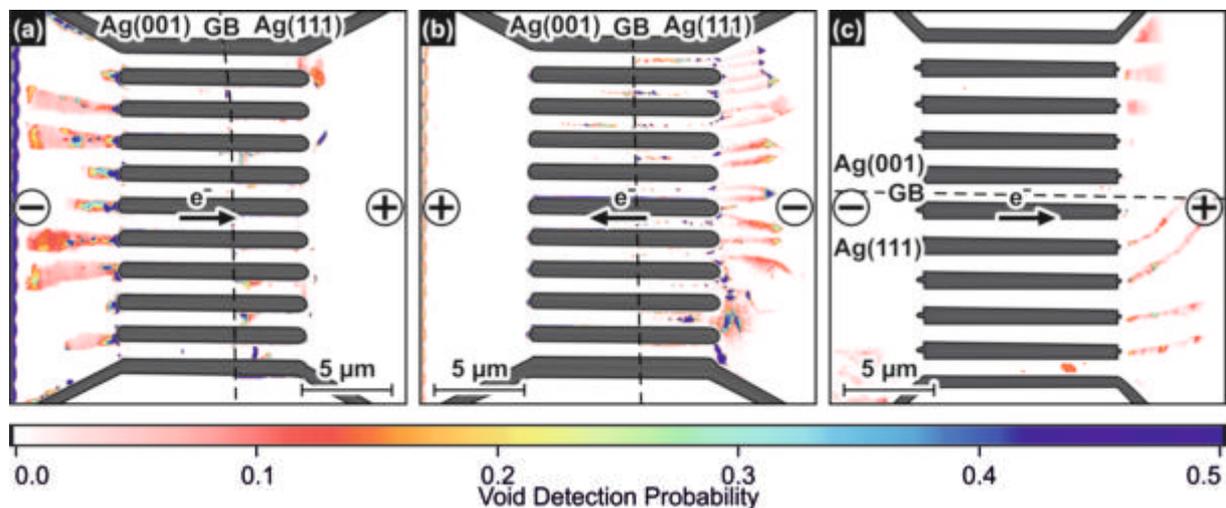
Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany

Due to the shrinking dimensions of interconnects below their mean grain size, diffusion mechanisms inside the grains become more important for electromigration (EM). We use well controlled bi-crystalline Ag test structures [1,2] to study the interaction of electromigration driven voids with the crystal lattice by in-situ scanning electron microscopy (SEM).

The influence of the lattice symmetry is strongly reflected in the void shape. In test structures with wires perpendicular to the GB, voids exhibit a triangular top view shape in the Ag(111) part and pronounced rectangular top view shapes in the Ag(001) part [3]. Once a void has passed through the crystal lattice, we observed an increased number of additional voids in the previous motion path [4]. Thus, the microstructure seems to remember the initial motion path.

For a test structure with a parallel GB (90° rotated), voids again exhibit triangular top view shapes in the Ag(111) part, but are rotated by 30°. Surprisingly, the motion direction of voids is also rotated by various angles between 20° and 60°. The motion direction of voids does not coincide with the EM force direction [4,5].

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**Fig. 1:** Void Maps of three different lattice: (a) Voids in the Ag(001) part with EM force in  $\langle 110 \rangle$  direction; (b) Voids in Ag(111) part with EM force in  $\langle 112 \rangle$  direction; (c) Voids in the Ag(111) part with EM force in  $\langle 110 \rangle$  direction. The color code represents the probability to find a void in any frame of the SEM image sequence at a given position.

**Notes**

# Charge storage in $\beta$ -FeSi<sub>2</sub> nanoparticles

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The increasing use of mobile electronics creates a steady demand for new energy storages with very high capacitance. Here we report on the observation of a surprisingly high specific capacitance of  $\beta$ -FeSi<sub>2</sub> nanoparticle layers.

Lateral, interdigitated capacitor structures were fabricated on thermally grown silicon dioxide and covered by FeSi<sub>2</sub> particles by drop or spin casting. The FeSi<sub>2</sub>-nanoparticles, with sizes in the range of 10-30 nm, were fabricated by gas phase synthesis in a hot wall reactor. Compared to the bare electrodes, the nanoparticle-coated samples exhibit a 3-4 orders of magnitude increased capacitance. Time-resolved current voltage measurements show that for short times (seconds to minutes), the material is capable of storing up to 1 As/g at voltages of around 1 V. The devices are robust and exhibit long term stability under ambient conditions. The specific capacitance is highest for a relative humidity of 95%, while for a relative humidity below 40% the capacitance is almost indistinguishable from a nanoparticle-free reference sample. The devices work without the need of a fluid phase, the charge storing material is abundant and cost effective, and the sample design is easy to fabricate.

**Notes**

# Preparation of BaTiO<sub>3</sub> sols suitable for films fabrication using a commercial inkjet printer

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Ink-jet printing is often used as one of the low cost methods for fabrication of ceramic thick films with broad application in microelectronics [1]. By ink-jet printing, droplets of a previously prepared sol (ink) can be deposited at predetermined locations on a substrate and after drying and thermal treatment desirable complex structures can be obtained. As it is well known that the sol characteristics determine the performances of the final product [2], this research is focused on preparation of different BaTiO<sub>3</sub> sols suitable for use in ink-jet printing. Stability of the sols with variation of the processing parameters was investigated.

BaTiO<sub>3</sub> sols were prepared by dissolving barium-carbonate in acetic acid and subsequent addition of tetrabutyl-orthotitanate. In addition, formamide and glycerin were added in the system in several concentrations to improve sol stability. Determination of viscosity, surface tension and particle size distribution, were used for the characterization of the precursor sols. The prepared sols were printed on previously cleaned substrates using a commercial ink printing device. After the drying and heating treatment continuous films were formed. Phase composition was determined by XRD analysis and the structure and morphology of the deposited films were evaluated by optical microscopy, scanning electron microscopy and EDS analysis.

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**Notes**

# Simulation of fractal abnormal grain growth in nanocrystalline materials

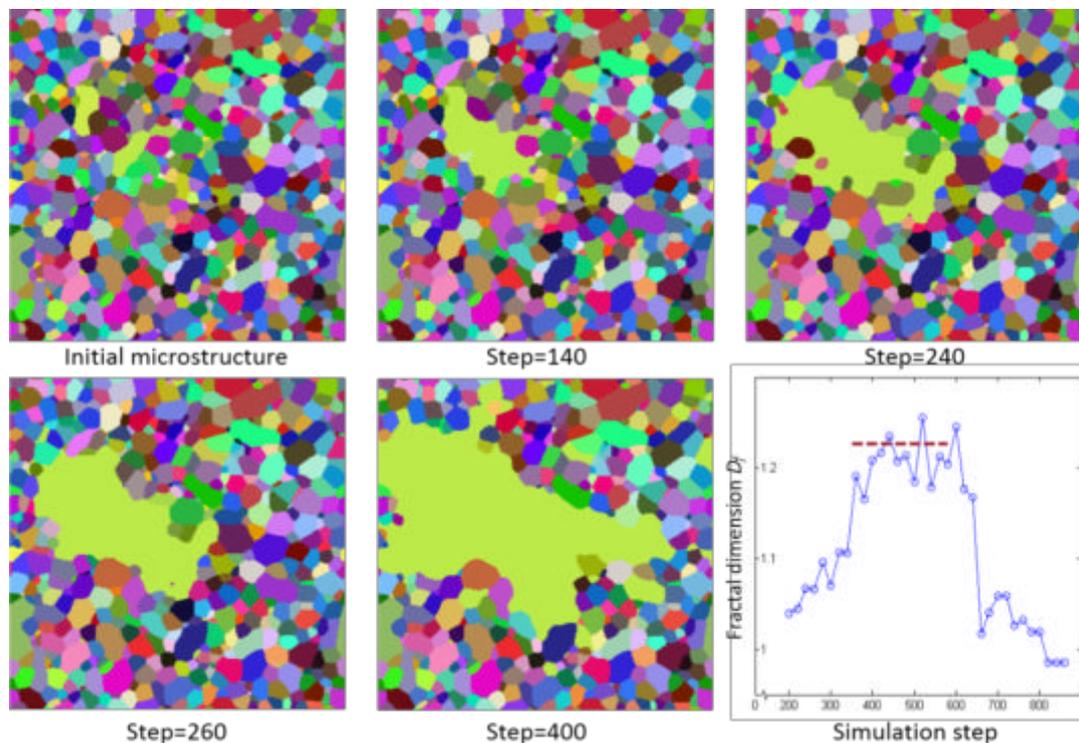
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Despite the rarity suggested by its name, abnormal grain growth (AGG) appears to be a common mode of coarsening in nanocrystalline specimens, observed in a wide variety of materials prepared by a range of synthesis routes. During AGG, a subpopulation of grains manifests rapid growth [1], leading to grain volumes that not only are much larger than those of their neighbors, but also are sometimes highly irregular in shape [2]. The nature of this irregularity can be described by the geometric concept of fractals [3]. This observation suggests that, in certain cases, AGG might proceed by some kind of percolation process taking place on the 'grid' defined by the initial ensemble of grains.

We have investigated this possibility by extending a conventional phase field algorithm for simulating grain growth to include selection rules for percolation (Fig. 1). For properly chosen parameter values, the abnormal grains generated by simulation can be strikingly similar in shape to their experimental counterparts. Quantifying the comparison between simulation and experiment, we hope to shed light on at least one of the underlying physical mechanisms for AGG in nanocrystalline materials.

- [1] F. J. Humphreys and M. Hatherly, *Recrystallization and Related Annealing Phenomena*, 2nd ed., Elsevier, Amsterdam, **2004**
- [2] M. Ames, J. Markmann, R. Karos, A. Michels, A. Tschöpe and R. Birringer, *Acta Mater.* **56** (2008) 4255–4266
- [3] B. B. Mandelbrot, *Fractals: Form, Chance, and Dimension*, *W. H. Freeman*, San Francisco, **1977**



**Fig. 1:** Simulation of a seed grain growing abnormally in 3D according to selection rules for percolation. Images show a cross-sectional slice through the seed grain at the indicated simulation step numbers. The fractal dimension of the perimeter of the abnormally growing grain increases initially and then takes on a constant value of  $D_f = 1.23 \pm 0.06$  (dashed line).

**Notes**

# Modeling of a cohesive, caking powder in DEM simulations

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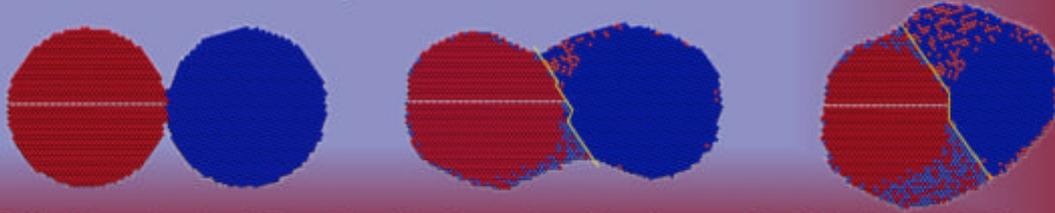
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As the capacity of modern computers increases, it has become feasible to do simulations of bulk solids with particle numbers close to those in real experiments. Capturing every detail, however, remains a challenge, especially when dealing with non-spherical, cohesive particles and a large particle size distribution. Using the the example of  $\mu\text{m}$ -sized potassium chloride (KCl), we will present an approach to model a cohesive, caking powder in DEM-Simulations. By calibration of an idealized ensemble of spheres, we are able to reproduce the macroscopic flow properties of KCl observed in experiments.

**Notes**



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MiFuN – Microstructural Functionality: Dynamics, Adaption, and Self-Healing at the Nanoscale



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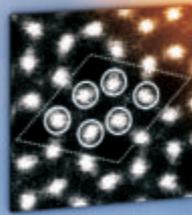
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