MiFun

Microstructural Functionality at the Nanoscale

Duisburg, Germany October 4th to 6th, 2017



UNIVERSITĂT DUISBURG ESSEN

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Program Overview

Wednesday, October 4, 2017

8:30	Opening	Markus Winterer
	3D Systems	chair: Roland Schmechel
08:45	Richard I. Todd, Oxford	
09:30	Olivier Guillon, Jülich	
10:45	Malte Jongmanns, UDE	
11:00	Claudia Gorynski, UDE	
11:15	Lukas Engelke, UDE	
	2D Systems	chair: Meyer zu Heringdorf
11:30	Jamie Warner, Oxford	
13:00	Juliana Morbec, UDE	
13:15	Bilge Bekdüz, UDE	
13:30	Rolf Möller, UDE	
13:45	Marika Schleberger, UDE	
	1D Systems	chair: Werner Prost
15:00	Erik Bakkers, TU Eindhoven	
15:45	Nils Benson, UDE	
16:00	Fangzhou Wang, UDE	
	3D Systems – 2	chair: Markus Winterer
16:45	Cahit Benel, KIT	
17:00	Christopher Schuh, MIT	

Thursday, October 5, 2017

	Advanced Characterization Matheda	oboir: Dolf Möllor
	Advanced Characterization Methods	
08:30	Florian Banhart, U Strasbourg	
09:15	Dmitry Turchinovich, UDE	
	Interface Functionality	chair: Christof Schulz
10:30	Bilge Yildiz, MIT	
11:15	Vladimir Srdic, U Novi Sad	
11:30	Benjamin Geisler, UDE	
11:45	Christian Blumberg, UDE	
13:00	Poster Session	
	Theory and Simulation	chair: Rossitza Pentcheva
14:00	Jerry Tersoff, IBM	
14:45	María José Caturla, U Alicante	
16:00	Kirk Bevan, McGill U	
16:30	Reza D. Kamachali, MPI / RUB	
17:00	Rajiv Kalia, USC	

Friday, October 6, 2017

	2D Systems – 2	chair: Michael Farle
08:30	Michel Barsoum, Drexel U	
09:15	Malte Behrens, UDE	
	Dynamic Functionality	chair: Dietrich Wolf
10:00	Wilfred van der Wiel, U Twente	
10:45	Elena Panchenko, U Tomsk	
11:15	Markus Gruner, UDE	
11:45	Conclusion	Pentcheva, Wolf, Winterer
13:15	Social Event (visiting thyssenkrupp Steel Europe AG) and	
	Conference Dinner (Faktorei)	

Front Cover Legend / Acknowledgement

The ZnO nanowires ('propeller' diameter about 1 µm, HRSEM image) on the front cover have been synthesized and analyzed by our bachelor students Birvan Dogan Karaduman, Aran Mohammed and Mohammed Ali Sheikh during their NanoEngineering bachelor project. They were tutored by our PhD students Alexander Levish and Sasa Lukic (Winterer group, see page 110).

MiFuN

Microstructural Functionality at the Nanoscale

Duisburg, Germany, October 4th to 6th, 2017

International Advisory Board

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Venue

Lecture Hall MD 162 University of Duisburg-Essen Lotharstr. 1, 47057 Duisburg

MiFuN – Microstructural Functionality at the Nanoscale

This international workshop is intended to foster the interdisciplinary exchange of ideas between researchers in engineering, physics and chemistry on microstructural dynamics. The topic of MiFuN is the time dependence of structural features at the nanoscale, a recent research development that is expected to have a strong impact on nanoscience and technology. Mechanisms for microstructural evolution range from the formation of defects, their transport, growth and transformation, to segregation, sintering and cooperative mechanisms including the controlled manipulation of grain boundaries and other microstructural elements in nanocrystalline materials. These mechanisms can lead to novel dynamic functionality, such as resistive switching or self-healing and are also determining the lifetime of nanostructured devices. In 2017 the focus will be placed on mechanisms in inorganic 1D and 2D systems.

Duisburg, October 2017

The local organizing committee

Markus Winterer, Nanoparticle Process Technology Dietrich Wolf, Computational and Statistical Physics Rossitza Pentcheva, Computational Materials Physics

University of Duisburg-Essen



Wednesday, October 4, 2017

08:00	Registration	
08:30	Opening	Markus Winterer
	3D Systems	chair: Roland Schmechel
08:45	Richard I. Todd, Oxford Flash sintering mechanism	
09:30	Olivier Guillon, Jülich Flash sintering experiments	
10:15	Coffee Break	
10:45	Malte Jongmanns, UDE Lattice defects due to nonthermal phonons – a possible r	nechanism for flash sintering?
11:00	Claudia Gorynski, UDE Pattern Formation During Current Sintering of Aluminium Doped Zinc Oxide	
11:15	Lukas Engelke, UDE Simulation of Pattern Formation during Current Sintering	
	2D Systems	chair: Meyer zu Heringdorf
11:30	Jamie Warner, Oxford Atomic Level Dynamics in 2D Systems	
12:15	Lunch Break	
13:00	Juliana Morbec, UDE Tailoring the electronic and magnetic properties of monol applied strain	ayer phosphorene by doping and
13:15	Bilge Bekdüz, UDE CVD growth of graphene at reduced temperatures	
13:30	Rolf Möller, UDE Reversible 2D Phase Transition driven by an Electric Field	
13:45	Marika Schleberger, UDE Ion interaction with Graphene	
14:30	Coffee Break	
	1D Systems	chair: Werner Prost
15:00	Erik Bakkers, TU Eindhoven Defects (and their dynamics) in Nanowires	
15:45	Nils Benson, UDE Modeling of electron beam induced GaAs nanowire attrac	ction
16:00	Fangzhou Wang, UDE Magnetic hardening of FeCo nanowire arrays at 300 K	
16:15	Coffee Break	

Wednesday, October 4, 2017 – continued

	3D Systems – 2	chair: Markus Winterer
16:45	Cahit Benel, KIT Cluster-assembled Metallic Glasses	
17:00	Christopher Schuh, MIT Design of Stable Nanocrystalline Alloys	
17:45	Informal Dinner	

Thursday, October 5, 2017

08:00	Registration	
	Advanced Characterization Methods	chair: Rolf Möller
08:30	Florian Banhart, U Strasbourg Ultrafast Electron Microscopy	
09:15	Dmitry Turchinovich, UDE Terahertz Physics of Graphene	
10:00	Coffee Break	
	Interface Functionality	chair: Christof Schulz
10:30	Bilge Yildiz, MIT Beyond Electrostatic Effects at Oxide Hetero-interfaces: Electrochemical Phase Change, Strong Electric Fields, and Elastic Strain	
11:15	Vladimir Srdic, U Novi Sad Interface effects in multilayer BaTiO ₃ /NiFe ₂ O ₄ thin films prepared by solution deposition method	
11:30	Benjamin Geisler, UDE Design of n- and p-type thermoelectrics in oxide superlattices exploiting interface polarity	
11:45	Christian Blumberg, UDE Maskless Selective Area Epitaxy of 3D-GaN on Si(111)	
12:00	Lunch Break	
13:00	Poster Session	
	Theory and Simulation	chair: Rossitza Pentcheva
14:00	Jerry Tersoff, IBM Nanowire growth	
14:45	María José Caturla, U Alicante Molecular Dynamics Simulations of Defect Production in Graphene by Carbon Irradiation	
15:30	Coffee Break	
16:00	Kirk Bevan, McGill U Capacitive Charging and Electromigration: A Quantum Transport Perspective with Hydrody- namic Analogues	
16:30	Reza D. Kamachali, MPI / RUB Stability of self-stressed precipitates in metallic alloys	
17:00	Rajiv Kalia, USC Petascale Simulations of Exfoliation in Layered Materials and Crack Healing in a Nanocom- posite	
17:45	Informal Dinner	

Friday, October 6, 2017

08:00	Registration	
	2D Systems – 2	chair: Michael Farle
08:30	Michel Barsoum, Drexel U A new deformation micromechanism in the deformation of layered solids: ripplocations	
09:15	Malte Behrens, UDE Topotactic Synthesis of Porous Cobalt Ferrite Platelets from a Layered Double Hydroxide Precursor and their Application in Oxidation Catalysis	
09:30	Coffee Break	
	Dynamic Functionality	chair: Dietrich Wolf
10:00	Wilfred van der Wiel, U Twente Evolution of a designless nanoparticle network into reconfigurable Boolean logic	
10:45	Elena Panchenko, U Tomsk Effect of Microstructure Evolution on Two-Way Shape Memory Effect in Aged Ni ₄₉ Fe ₁₈ Ga ₂₇ Co ₆ Single Crystals	
11:15	Markus Gruner, UDE Unraveling the formation of nano-twinned martensites in Ni ₂ MnGa magnetic shape memory alloys	
11:45	Conclusion	Rossitza Pentcheva Dietrich Wolf Markus Winterer
12:00	Lunch Break	
13:15	Bus leaving for	
-	Social Event (visiting thyssenkrupp Steel Europe AG) and Conference Dinner (Faktorei)	
22:00		



(Abstracts in order of appearance in the oral program; presenting author in bold)

Flash sintering of ceramics: what it is, what we know and what we would like to know

Richard Todd¹, E. Zapata-Solvas¹, B. Parker¹, S. Falco¹, S. Bonilla¹, M. Yoshida¹, W. Ji^{1,2}, J. Y. Zhang², Z. Y. Fu²

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² Wuhan University of Technology, PR China

"Flash sintering" refers to the rapid densification of ceramics at low furnace temperatures by passage of an electric current through the specimen and was first reported by Raj and co-workers in 2010 [1] using the ionic conductor 3 mol% yttria stabilised zirconia (3YSZ). Since then it has been demonstrated in many other ceramics. The low furnace temperatures, rapid turnaround times and possibilities of producing novel microstructures offer significant commercial advantages but controlling the process is essential as severe localisation of the temperature can occur under some conditions. In order to do this, the process needs to be understood so that that predictive process models can be developed.

In this presentation, the main features of flash sintering are illustrated. Areas where consensus is developing are highlighted along with areas where more information is needed. It is first shown that the thermal and electrical response during the flash event can be explained and modelled well in terms of classical thermal runaway of Joule heating resulting from the negative temperature coefficient of resistivity exhibited by most ceramics under the relevant conditions of high temperature and electric field [2]. Questions concerning the electrical conduction of ceramics under these conditions are highliahted.

The second part of the presentation concerns the origin of the rapid sintering observed. There is consensus that the passage of an electric current through the specimen leads to significant heating above the furnace temperature but simplistic extrapolations from conventional sintering experiments cannot explain the rapid sintering by this factor alone. Experiments are described in which 3YSZ powder compacts are heated and cooled with a temperature profile similar to that of flash sintering but without the application of an electric field [3]. The results show a significant acceleration in sintering rate compared with conventional sintering at the same temperature but without the involvement of electricity. It is concluded that the rapid heating in flash sintering rather than the electric current responsible for it is a major cause of the accelerated sintering observed, at least in 3YSZ. Possible explanations for this "ultra-fast firing effect" are discussed.

- R.I. Todd, E. Zapata-Solvas, R.S. Bonilla, T. Sneddon, P.R. Wilshaw, J. Eur.Ceram. Soc. 35 (2015) 1865–1877 [2] [3]
- W. Ji, B. Parker, S. Falco, J.Y. Zhang, Z.Y. Fu, R.I. Todd, J. Eur. Ceram. Soc. 37 (2017) 2547-2551

M. Cologna, B. Rashkova, R. Raj, J. Am. Ceram. Soc. 93 (2010) 3556-3559 [1]

Spark plasma sintering of ceramics revisited as water assisted sintering process

Olivier Guillon

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Field Assisted Sintering Technique / Spark Plasma Sintering offers the possibility of applying uniaxial mechanical pressure as well as high heating rates. Under low voltage conditions, the electric field effect is however most of the time negligible. With the presence of water added to the powder, FAST/SPS unveils new, attractive possibilities for the sintering of hydrophilic oxide materials at extremely low temperatures [1,2]. For example, it was possible to fully densify nanocrystalline ZnO at 250°C. Densification kinetics is dramatically enhanced in the presence of water or aqueous solution. Ultrafine microstructure can be retained for densities up to 99.5%. Defects were analyzed by different spectroscopic methods, and Kelvin probe force microscopy enabled the mapping of local changes in defect concentrations and properties of grain boundaries in contrast to grains. This leads to a better understanding of the mechanisms for water-assisted densification and the related lower activation energy.



- B. Dargatz et al. J. Eur. Ceram. Soc. 36 (2016, 1207
- [1] [2] B. Dargatz et al. J. Eur. Ceram. Soc. 36 (2016) 1221

Fig. 1: Sintering path (grain size as a function of relative density) for nanocrystalline ZnO (NG20) [2]

Lattice defects due to nonthermal phonons – a possible mechanism for flash sintering?

Malte Jongmanns and Dietrich E. Wolf

Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

Flash sintering is a method to densify green compacts in just a few seconds at much lower furnace temperatures than in conventional sintering methods [1]. In a typical flash sintering experiment, a specimen is heated under a DC electric field, and it is observed that the specimen's current increases abruptly at a critical power density, at which rapid densification happens. While flash sintering has been observed for multiple materials (for an overview, see for example [2]), the responsible mechanism of this phenomenon still remains controversial. One possible mechanism is the nucleation of lattice defects [3], which would offer an explanation for nearly all aspects of flash sintering. Yet, so far there is no evidence that lattice defects actually do nucleate during flash sintering.

We investigate the possibility of the nucleation of lattice defects during field assisted sintering with a simple toy model: We perform Molecular Dynamics simulations of an fcc crystal (with periodic boundary conditions along the **a**- and **b**-axis and a free surface) using a Lennard-Jones potential. The initial configuration is a single crystal. We assume that the current excites primarily one lattice vibration mode near the Brillouin-zone boundary with a given rate and random phases. As phonon thermalization is slow, this leads to a non-equilibrium distribution of lattice vibrations. Preliminary evidence is presented that defect creation is an important dissipation channel before the crystal melts.

- M. Cologna, B. Rashkova, R. Raj, J. Am. Ceram. Soc. **93** (2010) 3556 M. Yu, S. Grasso, R. Mckinnon, T. Saunders, M. J. Reece, Adv. Appl. Ceram. **116** (2017) 24 [2]
- [3] K. S. Naik, V. M. Sglavo, R. Raj, J. Eur. Caram. Soc. 34 (2014) 4063



Fig. 1: Formation of lattice defects after excitation of phonons near the Brillouin-zone boundary

Pattern formation during current sintering

Claudia Gorynski¹, Lukas Engelke², Malte Jongmanns², Dietrich Wolf² and Markus Winterer¹

¹ Nanoparticle Process Technology, Faculty of Engineering, and CENIDE, University of Duisburg- Essen, Duisburg, Germany ² Computational and Statistical Physics, Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

We observe pattern formation during current sintering of aluminum doped zinc oxide. The formation of bands perpendicular to the current direction occurs on the micrometer scale, much larger than the microstructure in the green body consisting of nanocrystalline particles [1]. Our hypothesis is that the pattern formation is due to a feedback between Joule heating and segregation of Al-Zn-spinel as an insulating phase in doped zinc oxide as conducting matrix. [2] We want to understand the underlying mechanism and control the pattern formation to either eliminate or minimize segregation or deliberate-ly generate tailored patterns.

Nanocrystalline aluminum doped zinc oxide is synthesized using Chemical Vapor Synthesis (CVS). Green bodies are formed by uniaxial compaction. They are current sintered with a systematic variation of electrical current and flow geometries. The resulting microstructures are investigated using HRSEM, EDX and XRD.

Aluminum is homogeneously distributed in the nanocrystalline zinc oxide particles after CVS although, thermodynamically, it is insoluble. Therefore, segregation and second phase formation is observed after sintering. Pattern formation occurs only during current sintering and not during thermal sintering.

We propose a feedback between the electrical current used for the Joule heating during sintering and the generation of an insulating phase as possible mechanism for the self-organized pattern formation.

D. Gautam, M. Engenhorst, C. Schilling, G. Schierning, R. Schmechel and M. Winterer, J. Mater. Chem. A 3 (2015) 189
S. Angst, G. Schierning and D. E. Wolf, AIP 593 (2013) 1542



Fig. 1: ZnO nanoparticles doped with 0.5% AI by Chemical Vapor Synthesis and current sintered at 900°C

Simulation of pattern formation during current sintering

Lukas Engelke and Dietrich E. Wolf

Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

Current activated sintering of nano-particle powders frequently leads to intriguing microstructure evolution, which differs remarkably from the well-known sinter kinetics in a furnace. The most relevant difference is probably that a fully dense specimen is obtained much faster and at lower average temperature than for the classical process, hence preserving the nano-cristallinity of the material. However, in powders with various components, it has also been observed, that the electrical current may lead to a heterogeneous microstructure [1]. An example are the striped patterns, which form in Aldoped ZnO during current sintering, see the left part of Fig. 1. The structural analysis reveals that the stripes are rich in spinel phase, which in contrast to the doped ZnO is insulating.

The microscopic mechanisms of current activated sintering are still controversial, although there is a high demand for a better understanding of the microstructure evolution. It would enable the design of the process protocol such that it leads to the desired outcome. We adapted a simulation model, we had developed for the study of thermoelectric materials [2,3], to the case of Al-doped ZnO. The model combines transport calculations with sinter and phase transition dynamics. The simulation results in patterns very similar to the experimental ones (see right part of Fig. 1). We explain this model and the mechanism, by which it leads to the stripes.

- [1] A. Sandmann, C. Notthoff, and M. Winterer, J. Appl. Phys. 113 (2013) 044310
- [2] [3] S. Angst, and D. E. Wolf, New J. Phys. 18 (2016) 043004
- S. Angst, L. Engelke, M. Winterer, and D. E. Wolf, EPJ Web of Conferences 140 (2017) 13014



Fig. 1: Left: Precipitation bands in Al-doped ZnO, courtesy of Christian Notthoff and Markus Winterer. Right: Our simulation of a model for the same pattern formation process due to current sintering. The current direction in both figures is from bottom to top.

Atomic structure of dislocations, grain boundaries, vacancies and dopants in monolayered materials

Jamie H. Warner

Department of Materials, University of Oxford, OX13PH Oxford, UK

Defects in 2D materials impact their properties and therefore developing an accurate understanding at the atomic level is crucial for improving the material quality and application. Aberration corrected transmission electron microscopy is one of the leading approaches to studying the atomic structure of 2D materials [1]. In this talk, I will present recent work on understanding the detailed bonding in monolayered transition metal dichalcogenides (TMDs), MoS₂ and WS₂, which are direct band gap semiconductors and effective catalysts for hydrogen evolution reaction (HER). Using annular dark field scanning transmission electron microscopy (ADF-STEM) enables the detection of individual atoms and their elemental discrimination. I will show how this was used to identify single metal substitutional Cr and V dopants in TMDs and their high temperature dynamics, figure 1 [2]. Results on grain boundaries (GBs) in polycrystalline TMDs will be presented, including resolving the structure of dislocations and the presence of nanopores at the GBs. Details of sulfur vacancies will be presented [3], showing how they rapidly diffuse at high temperature to form extraordinarily long line vacancies that act as 1D atomic channels for vacancy agglomeration. Insights into crack propagation in 2D materials with atomically sharp tips will be discussed and how dislocations interact with crack tips to mediate movement [4]. The structure of ultra-flat edges in TMDs at high temperatures is examined and revealed to have unique Mo terminations that lead to separation of spin transport channels in nanoconstrictions [5]. Finally I will present results on the atomic level insights into single Pt doped MoS₂ monolayers for HER applications, where the correlation between Pt binding sites and catalytic activity is explore in unprecedented detail [6], and then extended to epitaxial Pt nanoparticles on MoS₂[7]. The results here make use of in-situ heating holders with customized modifications as well as electrical biasing holders in the TEM to gain further knowledge about electrical breakdown [8], joule annealing and thermal processing. These results reveal how deviation from perfect pristine single crystals can be understood at the atomic level in 2D semiconducting materials grown by CVD that are used in current opto-electronic devices.

- [1] J. H. Warner, E. R. Margine, M. Mukai, A. W. Robertson, F. Giustino, A. I. Kirkland, Science 337 (2012) 209
- [2] A. W. Robertson, Y-C. Lin, S. Wang, H. Sawada, C. S. Allen, Q. Chen, S. Lee, G-D. Lee, J. Lee, S. Han, E. Yoon, A. I. Kirkland, H. Kim, K. Suenaga, J. H. Warner, ACS Nano **10** (2016) 10227
- [3] S. Wang, G-D. Lee, S. Lee, E. Yoon, J. H. Warner, ACS Nano 10 (2016), 5419
- [4] S. Wang, Z. Qin, G. S. Jung, F. J. Martin-Martinez, K. Zhang, M. J. Buehler, J. H. Warner, ACS Nano 10 (2016) 9831
- [5] Q. Chen, H. Li, W. Xu, S. Wang, H. Sawada, C. S. Allen, A. I. Kirkland, J. C. Grossman, J. H. Warner, Nano Létters 2017 articles ASAP.
- [6] H. Li, S. Wang, H. Sawada, G. G. D. Han, T. Samuels, C. Allen, A. I. Kirkland, J. C. Grossman, J. H. Warner, ACS Nano 11 (2017) 3392
- [7] S. Wang, H. Sawada, Q. Chen, G. G. D. Han, C. S. Allen, A. I. Kirkland, J. H. Warner, ACS Nano 2017 Articles ASAP
- [8] Y. Fan, A. W. Robertson, Y. Zhou, Q. Chen, X. Zhang, N. D. Browning, H. Zheng, M. H. Rummeli, J. H. Warner, ACS Nano 2017 Articles ASAP



Fig. 1: ADF-STEM imaging and single atom EELS of Cr substitutional dopant in MoS₂.

Tailoring the electronic and magnetic properties of monolayer phosphorene by doping and applied strain

Juliana M. Morbec¹, Gul Rahman², and Peter Kratzer¹

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Phosphorene is an intriguing two-dimensional material with potential for a variety of applications, including field-effect transistors, photodetectors, and energy storage. Its anisotropic optical and electronic properties combined with high carrier mobilities, negative Poisson's ratio and promising thermoelectric properties have attracted increasing attention in the past few years. Moreover, its superior mechanical flexibility (monolayer phosphorene can theoretically sustain tensile strain up to 30% [1]) has opened the possibility of tuning its electronic and magnetic properties. Using first-principles calculations based on density functional theory we investigate the effects of uniaxial and biaxial strain on the electronic and magnetic properties of pristine and Carbon-doped monolayer phosphorene. We find that compressive in-plane strain can reduce the band gap of pristine phosphorene and induce a semiconductor-metal transition; by varying the applied biaxial strain up to 10% we find that it is possible to switch from a direct semiconductor to an indirect semiconductor and eventually to a metal. Tensile strain is also found to increase the stability of magnetic single vacancy defects. C-doped phosphorene was predicted to be magnetic and metallic; our results show that compressive biaxial strain suppresses the magnetism whereas tensile strain leads to an increasing in the magnetic moment and to an opening of the band gap. Our findings suggest that applying strain is an important method to tailor the electronic and magnetic properties of monolayer phosphorene.

[1] Qun Wei and Xihong Peng, Appl. Phys. Lett. 104 (2014) 251915

CVD growth of graphene at reduced temperatures

Bilge Bekdüz, Jonas Twellmann, Yannick Beckmann, Jan Mischke, Wolfgang Mertin, Gerd Bacher

Werkstoffe der Elektrotechnik and CENIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany

An attractive method to produce large area graphene with good quality is chemical vapor deposition (CVD), which is considered as the most promising approach for industrially relevant fabrication. In thermal CVD, methane or alternative carbohydrates are dissociated at temperatures around 1000°C on copper, which is well studied in literature. However to grow graphene continuously, e.g. in a roll-to-roll process, the temperature must be reduced to avoid any liquidization of copper.

We use a commercially available 4" reactor for growing large area monolayer graphene. Studying the relation between growth rate and structure of graphene by varying the pressure and the methane to hydrogen ratio at 1020 °C, we show that at low growth rates the defect density and hence the sheet resistance can be lowered [1]. By reducing the temperature to 750°C, the growth rate decreases by about 5 orders of magnitude in thermal CVD (Fig. 1 a). Independent on the methane partial pressure, an activation energy of 6.5 eV is derived for the temperature dependent growth rate, which we mainly attribute to the energy needed for dissociating the precursor. For enhancing the growth rate at low temperatures, we deploy plasma to dissociate methane already in the gas phase. The plasma is induced by applying a pulsed DC voltage between two electrodes, on one of which the substrate is located. To suppress the influence of the electrical field on the substrate surface and to achieve lateral growth, we used a sacrificial copper foil as a faraday cage. With this process, a reduction down to 1.8 eV in activation energy and thus a three orders of magnitude increase in the growth rate at 800°C is observed. As can be seen in figure 1 b, the Raman spectrum of graphene grown with T-CVD at 800°C shows a multilayer signal and a pronounced defect peak, whereas graphene grown at the same temperature via PE-CVD is defect-free and exhibits monolayer behaviour.

[1] Bekdüz B, Beckmann Y, Meier J, Rest J, Mertin W and Bacher G, Nanotechnology 28 (2017) 185601



Fig. 1: Graphene growth at reduced temperatures a) Growth rate as a function of inverse temperature in thermal and plasma CVD b) Raman spectra of graphene grains grown by thermal and plasma enhanced CVD at $T = 800^{\circ}$ C.

Reversible 2D phase transition driven by an electric field

Ben Wortmann¹, Dennis van Vörden¹, Paul Graf¹, Roberto Robles², Paula Abufager^{2,3}, Nicolás Lorente⁴, Christian A. Bobisch¹, **Rolf Moeller**¹

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² ICN2 Catalan Institute of Nanoscience and Nanotechnology, CSIC and the Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain

³Instituto de Física de Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and Universidad Nacional de Rosario, Av. Pellegrini 250 (2000) Rosario, Argentina

⁴Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain

We report on a reversible structural phase transition of a two dimensional system which can be locally induced by an external electric field. [1] By means of scanning tunneling microscopy (STM) we determined two coexisting structural configurations of a CO monolayer on Cu(111): an α -phase (7 × 7 superstructure) and a β -phase (33 × 33) R30°. The balance between the two phases can be shifted by the electric field of the STM tip, causing the domain boundaries to move, increasing the area of the favored phase controllable both in location and size. If the field is further enhanced new domains nucleate. The arrangement of the CO molecules on the Cu surface is observed in real time and real space with atomic resolution while the electric field driving the phase transition is easily varied over a broad range. Our new manipulation mode permits us to bridge the gap between spontaneous long-range ordering of phase transitions and man-made CO structures created by molecular manipulation of CO adlayers [2,3]. Giving insight into the physics of structural phase transitions and facilitating the fabrication of arbitrary atomic patterns on tunable scale it is a promising route that needs to be explored.

- [1] B. Wortmann et al., Nano Letters 16 (2016) 528
- [2] A. J. Heinrich et al., Science **298** (2002) 1381
- [3] K. K. Gomes et al. Nature **483** (2012) 306



Fig. 1: top left: α -phase imaged at -0,4V, 50pA, top right β -phase imaged at 0,5V, 50pA. Bottom half shows the corresponding structures as calculated in DFT (grey: copper, yellow: oxygen, black: carbon). By applying an electric field, the phases can be switched reversibly.

Ion interaction with graphene and other 2D materials

Marika Schleberger

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Graphene as the first 2D material to be discovered by Geim and Novoselov somewhat more than a decade ago [1], has attracted attention from scientist and engineers ever since. Nowadays Graphene is but one of many 2D materials all of which have different and in part unique properties. These have inspired virtually hundreds of studies covering a wide range of interests, ranging from basic scientific aspects to novel and groundbreaking applications, for examples see [2]. Many of those studies have shown that graphene and other 2D materials are in fact as non-perfect as any other real solid, i.e. typically contain several types of defects [3] which significantly influence intrinsic properties such as mechanical strength [4], optical [5], or electronic properties [6]. This may or may not be advantageous for experiments and applications. Defects may thus either be exploited or, if unwanted but unavoidable, their detrimental influence on material properties needs to be well characterized.

Particle irradiation is a well-known tool for defect engineering and in particular ion irradiation may be used to introduce a wide range of defects with high precision by choosing the right irradiation conditions (ion type, energy, charge state, angle of incidence, fluence). While the damage mechanisms for electrons and singly charged ions with kinetic energies up to several keV are both well understood, this is not true for highly charged ions and swift heavy ions. Here, the damage is not due to binary collisions but is related to charge transfer, electronic excitations and ionization processes. As a consequence the effective energy deposition for these projectiles depends strongly on the target's material properties as well. In this context, 2D materials offer several advantages as a target material such as a well-defined thickness, different electronic properties to choose from, and last but not least facile handling and preparation procedures. Thus, 2D materials represent a novel approach to study the fundamental processes of ion-solid interactions and to proceed to a new level of control in defect engineering [7]. In my presentation I will present and discuss several examples (see fig.1) of defect engineering of graphene and other 2D materials via ion irradiation.

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Fig. 1: Examples of ion-induced defects in freestanding graphene (a,b) [7], freestanding MoS_2 (c) [7], and supported MoS_2 (d).

Bottom-up grown nanowire quantum devices

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InSb nanowires are used to detect first signatures of quasi particles called Majorana fermions. [1] Recently, different schemes for preforming braiding operations and uncovering the non-Abelian statistics of Majorana fermions are proposed. [2] Such operations are fundamental for topological quantum computing. For a universal computational architecture the realization of a near-perfect nanowire network assembly is needed in which Majorana states are coherently coupled.

Here, we demonstrate a generic process [3] by which we can design quantum circuits and more particularly any proposed braiding device by manipulating an InP substrate and thereby the nanowire growth position and orientation. This approach combines recent advances in materials growth and theoretical proposals. Our method leads to highly controlled growth of InSb nanowire networks with single crystalline wire-wire junctions. Additionally, nanowire "hashtag" structures are grown with a high yield and contacted. In these devices, the Aharonov–Bohm (AB) effect is observed, demonstrating phase coherent transport. These measurements reveal the high quality of these structures. This generic platform will open new applications in quantum information processing. Furthermore, these structures are well suited for epitaxial superconductor (SC) island growth. Superconductors can be grown epitaxially covering the full length of a wire facet. In order to measure the induced superconductivity properties, part of a superconductor should be removed. Using a design of trenches by manipulating the wire position on the trenches one wire can be used as a shadowing object for another wire.

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Modeling of electron beam induced GaAs nanowire attraction

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Scanning electron microscope (SEM) induced nanowire (NW) attraction or bundling is a well-known effect, which is mainly ascribed to growth parameters or material dependent properties [1, 2]. However, there have also been recent reports of electron beam induced nanowire bending by SEM or TEM imaging [3], which is not fully explained by the current models, especially when considering the electro-dynamic interaction between NWs.

With this contribution [4] we aim to help advance the understanding of this phenomenon, by introducing an electro-dynamic model based on capacitor and Lorentz force interaction, where the active NW bending is stimulated by an electromagnetic force between individual wires. The model includes geometrical, electrical and mechanical NW parameters, as well as the influence of the electron beam source parameters and is validated using in-situ observations of electron beam induced GaAs nanowire (NW) bending by SEM imaging.

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(a) Initial position (b) NW movement (c) Final position

Fig. 1: SEM induced NW displacement: a) Initial position prior to movement using a low image quality. b) With enhanced image quality NW movement occurs, generating the highlighted image artefacts. c) Final NW position after the SEM induced movement.

Magnetic hardening of FeCo nanowire arrays at 300 K

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Magnetic nanowires (NWs) are currently considered as potential candidates for alternative rare-earthfree permanent magnets, magneto-electric logics or memory storage units [1-2]. Exploiting the large shape anisotropy of 3d-metal NWs yields a large magnetic energy product, i.e. high remanent magnetization (MR) and large coercive field (HC). It has been shown recently that MR and HC can be significantly enhanced at low temperatures by oxidizing FeCo NW tips [2].

Here we explore the possibility of magnetic hardening of $Fe_{30}Co_{70}$ NWs at room temperature by interfacing their tips with antiferromagnetic Fe50Mn50 layers. For this purpose, $Fe_{30}Co_{70}$ NWs with diameter 40 nm and length 16 µm were grown in Anodic Aluminum Oxide (AAO) membranes. Both tips of NWs are opened by chemical etching the AAO membrane and AFM $Fe_{50}Mn_{50}$ was deposited by magnetron sputtering forming a sandwich structure (Fig. 1a). As a result (Fig. 1b), the enhancement of MR and HC are 24% and 49% at room temperature, respectively [4].

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Fig. 1: a) Top view SEM image of the NW tips covered with a Fe₅₀Mn₅₀ film. b) Magnetic hysteresis after different processing steps at room temperature.

Cluster-assembled metallic glasses

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Contrary to rapidly quenched metallic glasses, cluster-assembled metallic glasses (CAMGs) have precisely controlled building blocks in terms of their chemical composition and cluster size [1]. Our state-of-the-art cluster ion beam deposition (CIBD) system allows us to deposit various CAMG films under well-defined conditions with a precise control over cluster size. Furthermore, various compaction scenarios can be realized by varying the impact energies of the clusters [2,3].

A series of amorphous FeSc samples, with an average cluster size of 1000 atoms per cluster (according to TOF-MS analyses) were deposited onto substrates with impact energies of 0.05, 0.1, 0.2, 0.5, and 12 keV per cluster. From the initial TEM and XRD investigations, it is evident that the samples are fully amorphous. As Figure 1 indicates, the magnetic properties of the CAMG samples can be tailored by the impact energy, which affects the ferromagnetic to paramagnetic transition temperature. In order to prevent the samples from oxidation, the films are protected by 200 nm thick Mg capping layers. No evidence of oxidation is found by the X-ray absorption fine structure (EXAFS and XANES) spectroscopy analyses at the Sc and Fe K-edges. The distinct difference in magnetism of chemically identical amorphous alloys is an evidence for a novel atomic structure existing in cluster-assembled glasses and can provide a fundamental understanding of the structure-material property relation for CAMGs.

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Fig. 1: Zero field cooled/field cooled (ZFC/FC) magnetization measurements of cluster-assembled FeSc thin films, prepared with different impact energies and a cluster size of 1000 atoms per cluster.

Design of stable nanocrystalline alloys

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When the grain size of a metal is refined to a scale on the order of just a few nanometers, its strength, hardness, wear resistance, and other properties improve in dramatic ways. There is therefore significant interest in designing and deploying such nanocrystalline alloys for structural applications. However, refining the grain structure is a struggle against equilibrium, and nanocrystalline materials are often quite unstable; the grains grow given time even at room temperature, and the associated property benefits decline over time in service. In this talk, our efforts to design stable nanocrystalline alloys will be described. We rely on selective alloying as a method to lower the energy of grain boundaries, which can bring a nanocrystalline structure closer to equilibrium. This talk will highlight the path from theory, to proof-of-concept laboratory demonstration, to scale-up and commercialization of such alloys. Beginning from early successes with nanocrystalline alloy coatings, the talk will also outline future opportunities in bulk net-shape products and additive manufacturing. The prospects of stable nanocrystalline metals in a wide variety of applications will be described, including as substitute materials to reduce cost and cost volatility, as greener alternatives to legacy technologies, as next-generation structural materials with large performance increments over incumbent metals, and as an enabler of new 3D printing technologies.

Ultrafast electron microscopy

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Transmission electron microscopy (TEM) with continuous electron beams has excellent spatial but poor temporal resolution. This is due to the weak electron beam current of the order nanoamperes that doesn't allow collecting enough electrons within a very short time to record images, diffraction patterns, or electron energy-loss spectra. This limitation has been overcome by the technique of ultrafast TEM (UTEM) where short and intense electron pulses are generated by sending laser pulses onto a photocathode. This allows studying short-lived transient states in matter at the spatial scale of nanometers.

UTEM is carried out in a pump-probe approach, where a dynamic process in the object is induced by a laser pulse (pump), followed by another laser pulse which generates the electron pulse (probe) for imaging. Two complementary techniques of UTEM have been developed in the past decade. The single-pulse mode [1], where one intense electron pulse provides the whole information, is used for studying irreversible transformations. Reversible transformations can be studied in a stroboscopic mode where trains of weaker electron pulses are used [2]. The limiting factor in UTEM is the mutual repulsion of electrons within a pulse, leading to spatial, temporal, and energy broadening of the electron pulse.

A new UTEM, combining both the single-pulse and the stroboscopic mode in one instrument, has recently been launched at the University of Strasbourg. Detailed studies of the electron pulses have been undertaken to find the optimum operation conditions and the resolution limits [3]. The stroboscopic mode, where fewer electrons are in one pulse (less than 105) and repulsion effects are less important, allows sub-nanometer spatial and picosecond temporal resolution. Electron energy-loss spectra (EELS) can be taken with almost sub-eV resolution. In the single-pulse mode, up to 109 electrons have to be compressed into one pulse, and broadening effects are severe. Nevertheless, a spatial resolution of tens of nanometers is attained when the temporal length of the pulses (given by the duration of the laser pulses) is of the order nanoseconds. For the first time, EEL spectra could be taken in the single-pulse mode, and a reasonable energy resolution of a few eV was reached. This shows the potential of UTEM in the single-pulse mode and the possibility to study irreversible chemical transformations by EELS with nanosecond resolution. A detailed overview of the achievements in the stroboscopic as well as in the single-pulse mode will be given.

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Terahertz physics of graphene

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In this presentation we will show, that the terahertz (THz) linear, non-linear and photo-conductivity of graphene [1–3] can be accurately described within a simple picture, in which the free carrier population of graphene acts as thermalized electron gas in or out of equilibrium with graphene lattice.

Within this thermodynamic picture, the electron population quasi-instantaneously increases its temperature by absorbing the energy of driving THz electric field or incident photon, and at the same time cools down via a time-retarded, few picosecond-long process of phonon emission. The asymmetry in electron heating and cooling dynamics leads to heat accumulation in the electron population of graphene, concomitantly lowering the chemical potential for hotter electrons, and thereby reducing the intraband conductivity of graphene – an effect crucially important for understanding of the performance of ultrafast graphene transistors and photodetectors.

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Beyond electrostatic effects at oxide hetero-interfaces: Electrochemical phase change, strong electric fields, and elastic strain

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Transition metal oxide hetero-interfaces are interesting due to the distinctly different properties that can arise from their interfaces, such as superconductivity, high catalytic activity and magnetism. These interfaces are the source for local heterogeneities in composition, atomic structure and electronic structure. Classically, defect redistribution is quantified at the continuum level by concurrent solution of Poisson's equation for the electrostatic potential and the steady-state equilibrium drift-diffusion equation for each defect. It is possible to inform this level of modeling with first principles calculations of band off-sets, and defect formation and segregation energies at thermodynamically relevant conditions. This approach had numerous successful implementations, including the quantification of charge transport properties at surfaces and grain boundaries. In this talk, I will discuss three phenomena that also need to be considered in a broader framework of defect structures and distributions at oxide hetero-interfaces. 1) Presence of strong electric fields that can cause polarization of defective systems and affect the defect abundance and structure. We have assessed this effect on neutral oxygen vacancies in simple binary oxides from first principles calculations. 2) Phase change under the effect of local electrostatic potential because of a change in the electrochemical potential of oxygen. We have assessed the ability to trigger phase change electrochemically in two classes of oxides, SrCoOx and VO_{x_1} and have quantified the phases and the corresponding distinctly different electronic properties by combining in operando x-ray diffraction and x-ray photoelectron and absorption spectroscopy. The results have implications both for oxide hetero-interfaces and for oxide electronic devices that aim to control properties electrically, 3) Elastic strain, that affect the stability and mobility of defects. In this recent work, we have focused on the stability of electronic defects, specifically the electron polarons versus free electrons SrTiO₃, as a function of temperature and hydrostatic stress, by combining first principles calculations and quasi harmonic approximation. Our results demonstrate that it is possible to control the type of electronic defect, and so the transport properties, by means of electro-chemomechanics.

Structure and functional properties of multiferroic $BaTiO_3/NiFe_2O_4$ multilayer thin films prepared by solution deposition technique

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Improving trend of microelectronic devices performance has led to new discoveries in field of material science. A novel group of materials, called multiferroics, have found a place in spotlight of scientific research because of their unique ability to exhibit more than one ferroic property. What is more important, coupling between ferroic properties is very attractive for different applications. In past few years, the concept of multiferroic tunel junctions, based on multilayer multiferric thin films, has opened a whole new direction of research, and potential application of multiferroics in resistive switching devices.

In this research the connections between structure and properties (dielectric, ferroelectric and ferromagnetic) of multilayer $BaTiO_3/NiFe_2O_4$ (BT/NF) thin films are presented. The multiferroic thin films were obtained by spin coating of ferroelectric and ferromagnetic layers in alternating order on platinum coated silicon substrates. Sintering was performed at different temperatures up to 1000 °C. All the obtained samples have the thickness below 600 nm (12 deposited layers at most), with defined ferrite and titanate layers, flat and crack-free surface. Low values of dielectric constant and polarization are in agreement with the microstructure on nanoscale, showing the presence of interface polarization. Magnetic measurements confirmed decrease of magnetization with presence of ferroelectric titanate layers in comparison to the pure NF films, but also indicated on mechanical straining between titanate and ferrite layers. In addition, I-V measurements of three layered BT/NF/BT films showed memristive behavior.

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Design of n- and p-type thermoelectrics in oxide superlattices exploiting interface polarity

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Transition metal oxides receive increasing attention for thermoelectric applications like waste-heat recovery due to their chemical and thermal stability and environmental friendliness. Advances in layerby-layer fabrication techniques have made it possible to fabricate epitaxial oxide superlattices with atomic precision, thereby providing a way to improve and/or tailor their thermoelectric properties.

We combine density functional calculations including an on-site Coulomb repulsion term and Boltzmann transport theory to explore the implications of the interface-dependent polar discontinuity in LaNiO₃/SrTiO₃(001) superlattices on the structural, electronic, and thermoelectric properties. While a $(LaO)^+/(TiO_2)^0$ stacking at the interfaces results in an *n*-type superlattice, a $(NiO_2)^-/(SrO)^0$ stacking leads to *p*-type doping. We find that significant octahedral tilts are induced in the SrTiO₃ region and that the La-Sr distances act as a fingerprint of the interface type. In contrast to the paradigmatic LaA-IO₃/SrTiO₃(001) system, the electrostatic doping is mainly accommodated in the metallic nickelate layers. The electronic structure displays an orbital-selective quantization of Ni-3*d*-derived quantum well states. Complex cylindrical Fermi surfaces emerge, which show a tendency towards nesting that depends on the interface polarity. Finally, we demonstrate that the thermoelectric response of the superlattice (i.e., the sign of the Seebeck coefficient) can be selectively controlled by a targeted interface design. This opens a route for constructing oxide-based thermoelectric generators [1, 2].

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Fig. 1: LaNiO₃/SrTiO₃(001) superlattices with *n*-type (left) and *p*-type (right) thermoelectric properties.

Maskless Selective Area Epitaxy of 3D-GaN on Si(111)

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Selective Area Epitaxy (SAE) of GaN on Silicon substrates is of high current interest due the electrical conductivity of the substrate, facilitating electrical contact schemes. In common SAE-methods dielectric masks and multiple growth runs for AIN/Si-templates and GaN-growth are needed.

In this work we present a new maskless SAE-method for 3D-GaN on Si (111) by a sitecontrolled growth using periodically ordered holes in the Si-surface. The holes are realized by nanoimprint and ex-situ etching processes. An AIN-intermediate-layer has to be grown on Si as a Gablocking layer. In one MOVPE-run, a surface-conform and thin (< 20 nm) AIN-layer and 3D-GaN structures were grown. The AIN growth temperature was identified as the critical factor for achieving sitecontrolled growth of GaN.

Temperatures above 930°C lead to inhomogeneous growth on top of the holes and inbetween. For 930°C dominant growth of GaN occurs only on top of the holes. Unexpected pits and surface topologies, appearing on the Si-surface during heat up for AIN-growth at high temperatures, have been identified as causes for unwanted nucleation sites. These pits are caused by hydrogen involved Si-etching. Furthermore KOH(aq) etch experiments reveal that GaN on any surface topology is unipolar. Since the growth rate strongly depends on the polarity, SAE of 3D-GaN could be achieved. This is an important feature for future rod-based opto-electronic devices.

Effect of nanoscale features on growth of semiconductor nanowires

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Semiconductor nanowires with diameters down to a few nm are readily grown from metal catalyst particles via the vapor-liquid-solid (VLS) process. This is traditionally pictured as a simple continuous process, but often the reality is much richer and more dynamic. The combination of in-situ UHV transmission electron microscopy with theoretical modeling has made it possible to understand many features of the nanoscale structure and dynamics. For example, the liquid catalyst droplet can jump from one facet to another during the growth process, with important consequences for dynamic stability and wire morphology [1]. Also the shape of the growth interface can oscillate during growth [2,3].

These dynamical aspects of the growth can have unexpected consequences for nanowire structure. In particular, nanowires of many III-V semiconductors can grow in either the zincblende or wurtzite crystal structure, and the reasons have been debated for years. Only recently was it found that the phase selection was directly coupled to the interfacial structure. The interface exhibits different growth dynamics in the two cases, which together with theoretical modeling enabled a clear picture of the underlying mechanism controlling phase selection [4].

Nanowires can grow from either solid or liquid catalysts, and the growth dynamics depend sensitively on the structure of the catalyst particle. AuSi catalysts exhibit unique surface phase transitions [5], and we have studied these using in-situ UHV transmission electron microscopy, and modeled them theoretically [6]. We find rich behavior with direct impact on the growth dynamics, as well as providing new insight into the thermodynamics of the surface phase transition.

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Molecular dynamics simulations of defect production in graphene by irradiation

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Out-of-plane displacements in suspended graphene play a significant role in many of its properties, in particular, its elastic and mechanical properties [1-3]. In fact, several authors have proposed that the properties of graphene could be modified by externally changing these ripples either through the addition of defects or by applying a compressive or a tensile strain [1,4]. In this work we first discuss the relationship between out-of-plane displacements and the elastic properties of graphene (Young's modulus and Poisson ratio) by performing molecular dynamics simulations of free-standing graphene under tensile load at different temperatures. Two of the most widely used interatomic potentials for graphene have been employed in these calculations, the AIREBO [5] and Tersoff [6, 7] potentials. We will discuss how point defects modify both the Young's modulus and the Poisson ratio, focusing in particular on the possible auxeticity behavior of graphene under certain conditions [8-10].

We will then analyze the type of defects produced by ion irradiation at different doses and initial strain conditions, from an initial tensile strain of 0.25% to a compressive strain of -0.25%. We show that the roughness of the graphene membrane is heavily modified by the irradiation, removing the randomness of the ripple distribution existing before irradiation. The effect of irradiation on the elastic properties of graphene is then analyzed by simulating two different ways of obtaining the Young's modulus: a tensile test and a nanoindentation simulation. The two methods and results are discuss and compared to existing experimental and simulation data [11-12].

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Capacitive Charging and Electromigration: A Quantum **Transport Perspective with Hydrodynamic Analogues**

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With current densities continuing to rise, further control over electromigration is vital to the sustained development of integrated circuit technology possessing high reliability. Moreover, an understanding of the forces driving electromigration is essential to achieving such engineering control [1,2,3]. In this talk we will explore how the process of charging a capacitor, and the resulting force which develops over time, can be understood in similar terms to electromigration. By slowing bringing the capacitive plates together from the tunneling through to the quantum conductance limit [1], a gradual transition in forces from the capacitive charging regime to the resistivity dipole limit is demonstrated [4,5]. Through a first-principles analysis of the forces during this transition it is argued that qualitative interpretations of electromigration might be more intuitively set in terms of classical hydrodynamic analogues (rather than independent "wind" and "direct" force descriptions [6]). In general, this work aims to further the development of both an intuitive semi-classical description of electromigration and a methodology to quantitatively engineer electromigration from first-principles.

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Stability of self-stressed precipitates in metallic alloys

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Diffusion-controlled precipitation on the nanoscale features in numerous structural and functional materials. Often this phase transformation is accompanied with internal stresses due to structural mismatch between the precipitate and the matrix phase that influence process of precipitation and ultimate properties of the mixture. In this work the interplay between diffusion process and stresses around the precipitates are studied. I introduce a chemomechanical coupling as a result of (solute) composition decency of the local stiffness in the system and report about its effects on the stabilization and arrangement of the precipitates [1-4]. The results are deduced from large-scale phase-field modelling and simulations of δ' precipitate in Al-Li system. A new mechanism of inverse ripening and self-arrangement of the precipitates are discovered [1, 2]. The results can have wide applications in microstructure and alloy design.

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Fig. 1: The radii of precipitates are shown over the course of simulations. Chemomechanical coupling results in inverse ripening of the precipitates. Black lines show average precipitate size. κ represents the rate of dependency of the elastic constants on the solute composition. $\kappa = a.i.$ are anisotropic coupling values.

Petascale simulations of exfoliation in layered materials and crack healing in a nanocomposite

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This presentation will focus on massively parallel molecular dynamics simulations of two- dimensional (2D) layered materials and a nanocomposite capable of sensing and repairing damage in high temperature/high pressure operating conditions. We have examined atomistic mechanisms underlying liquid-phase exfoliation of 2D materials and strain- induced structural phase transformations in a 2D alloy. I will also describe crack healing and grain-growth mechanisms in a composite consisting of silicon carbide/silica nanoparticles embedded in an alumina matrix.

A new deformation micromechanism in the deformation of layered solids: ripplocations

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Plastically anisotropic/layered solids are ubiquitous in nature and understanding how they deform is crucial in geology, nuclear engineering, microelectronics, 2D solids among many other fields. It has long been assumed that basal dislocations are the operative micromechanism occurring during the deformation of layered solids. Recently, however, a new defect termed a ripplocation - best described as an atomic scale ripple - was proposed to explain deformation in two-dimensional solids. In this talk I will leverage atomistic simulations of graphite to extend the ripplocation idea to bulk layered solids, and confirm that it is essentially a confined buckling phenomenon. In contrast to dislocations, bulk ripplocations have no Burgers vectors or polarities. In graphite, ripplocations are attracted to vacancies and other ripplocations, both within the same, and on adjacent layers, the latter resulting in kink boundaries. The latter form spontaneously when loaded. Furthermore, direct TEM evidence for bulk ripplocations in Ti₃SiC₂, a MAX phase layered carbide. The nucleation of delamination cracks, when atomic layers are loaded edge-on with, say, a spherical indenter, is one unambiguous signature of ripplocations. Ripplocations are not only a fundamentally new deformation micromechanism in the deformation of solids, but are a topological imperative, since it is the only way atomic layers can glide relative to each other without breaking the all-important in-plane bonds. A more complete understanding of their mechanics and behavior is critically important, and could profoundly influence our current understanding of how graphite, layered silicates - important in geology - the MAX phases, 2D solids and many other plastically anisotropic/layered solids, deform and accommodate strain.



Fig. 1: Atomistic molecular dynamics simulations of z-displacement in graphite at 10 K when indented with a 50 nm cylindrical indenter (top) with axis along y-direction. The deformation is initially linearly elastic; beyond a critical stress, ripplocations and kink boundaries of opposite polarities form spontaneously and are fully reversible.

Topotactic synthesis of porous cobalt ferrite platelets from a layered double hydroxide precursor and their Application in oxidation catalysis

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Monocrystalline, yet porous mosaic platelets of cobalt ferrite, $CoFe_2O_4$, can be synthesized from a layered double hydroxide (LDH) precursor by thermal decomposition. Using an equimolar mixture of Fe^{2+} , Co^{2+} and Fe^{3+} during co-precipitation, a mixture of LDH, $(Fe^{II}Co^{II})_{2/3}Fe^{III}_{1/3}(OH)_2(CO_3)_{1/6} \cdot m H_2O$, and the target spinel $CoFe_2O_4$ can be obtained in the precursor. During calcination, the remaining Fe^{II} fraction of the LDH is oxidized to Fe^{III} leading to an overall Co^{2+} : Fe^{3+} ratio of 1:2 as required for spinel crystallization. This pre-adjustment of the spinel composition in the LDH precursor suggests a topotactic crystallization of cobalt ferrite and yields phase pure spinel in unusual anisotropic platelet morphology. The preferred topotactic relationship in most particles is $[111]_{Spinel}||[001]_{LDH}$. Due to the anion decomposition, holes are formed throughout the quasi monocrystalline platelets (Fig. 1). This synthesis approach can be used for different ferrites and the unique microstructure leads to unusual chemical properties as shown by the application of the ex-LDH cobalt ferrite as catalyst in the selective oxidative dehydrogenation to acetone, the main reaction over the novel ex-LDH cobalt is dehydration to propene. Moreover, the OER activity of the ex-LDH catalyst was markedly higher compared to the commercial material [1].

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Fig. 1: SEM micrograph of the calcined LDH precursor showing aggregates of porous platelets (a) and HAADF-STEM image of one individual platelet (b).

Evolving functionality in disordered nanoscale networks

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Natural and man-made information processing systems differ greatly. Evolution has resulted in living systems that utilize whatever physical properties are exploitable to enhance the fitness for survival. Nature thereby exploits the emergent properties and massive parallelism of highly interconnected networks of locally active components. Man-made computers, however, are based on circuits of functional units, following rigid design rules. Hence, in conventional computational paradigms, potentially exploitable physical processes to solve a problem, are left out. We here propose evolution-in-materio, which mimics Darwinian evolution by manipulating physical systems using computer-controlled evolution, to take full advantage of the computational power of nanomaterials.

We have experimentally demonstrated that a designless network of gold nanoparticles acting as single-electron transistors, exhibits strongly non-linear behavior, which can be evolved into computational functionality. We have realized Boolean logic gates [1], and we plan to realize more advanced functionality such as pattern recognition. The viability of our approach is underlined by simulations based on both physical [2] and neural-network models [3]. Recent experimental results show that the above principle is generic, and can be demonstrated in other material systems as well, also at higher temperature.

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Fig. 1: Schematic representation of the disordered nanoparticle network. The inputs V_{in1} and V_{in2} are used for applying voltage input signals, the current output is measured at lout. The contacts V_1 - V_6 are used for applying control voltages, affecting the input-output characteristics.
Effect of microstructure evolution on two-way shape memory effect in aged Ni₄₉Fe₁₈Ga₂₇Co₆ single crystals

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Ferromagnetic shape memory alloys such as NiFeGaCo, have been extensively studied during the last years as they demonstrate large potential for use as thermal- and magnetic-controlled actuators and sensors for various applications [1, 2]. The two-way shape memory effect (TWSME) can be used for reversible changing size of actuator working element induced by the temperature and magnetic fields without any biasing force as compared to one-way shape memory effect [1]. In this study the efficiency of isothermal trainings (100 cycles loading/unloading) for inducing and cyclic stability of the TWSME depending on microstructure evolution in [001]-oriented ferromagnetic Ni₄₉Fe₁₈Ga₂₇Co₆ (ar. %) single crystals were investigated. On the basic of single crystals the nanostructured composites containing two types of particles are created by different thermo-mechanical treatment (annealing at 1373 K followed by quenching; stress-free and stress-induced aging at 673K for 4h). Particles of γ (A1)- and γ' (L1₂)-phases do not undergo martensitic transformation and are in size of 5 - 10 μ m and 10 - 30 nm (Fig. 1), respectively. Maximum reversible TWSME strain up to 5.5% was observed in stress-assisted aged single crystals in which the favorably oriented internal stress fields are created by the selection of certain y'-phase nanoparticle variants during stress-assisted aging and the oriented alignment of dislocations associated with anti-phase boundary is formed by training procedure. In quenched and stress-free aged crystals TWSME strains are less than 2.2%. The mechanisms of cycling degradation of TWSME (decrease of TWSME strain and changing in martensitic start temperature) have also been discussed. In guenched single crystals 100 thermal cycles results in irreparable degradation of TWSME. Whereas in contrast the age hardening in stress-free and stress-assisted aged crystals conduces unchanged martensitic start temperature during thermal cycles and the restoration of the TWSME strain due to additional training.

This work was supported by the Russian Science Foundation (grant No. 16-19-10250).

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Fig. 1: Residual martensite and nanoparticles of γ '-phase in stress-free aged Ni₄₉Fe₁₈Ga₂₇Co₆ single crystal after iso-thermal 100 cycles loading/unloading.

Unraveling the formation of nano-twinned martensites in Ni₂MnGa magnetic shape memory alloys

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The magnetic shape memory Heusler compound Ni2MnGa exhibits large strains of 10% in moderate magnetic fields of around 1 T at ambient conditions [1], which is of technological interest for actuator and sensor applications. Its unique functional properties are linked intimately to the presence of hierarchically twinned modulated structures. These can be interpreted in terms of an adaptive, selforganized arrangement of [110] aligned nano-twins consisting of tetragonal, non-modulated L10 building blocks [2,3]. The transformation path from cubic austenite to nano-twinned martensite is essentially downhill, which can be traced back to a pronounced shear anomaly in [110] direction arising from a electronic band-Jahn-Teller-type reconstruction of the Fermi surface which in particular softens the [110] transversal acoustic phonons [4,5]. Based on comprehensive total energy calculations in the framework of density functional theory, we demonstrate that the energy of nano-twinned microstructures can be decomposed into the contribution from the L10 volume fraction, the bare twin interface energy and the interaction between two neighboring interfaces at a given separation [6]. The interaction between the twins can be attractive, leading to a competition between non-modulated tetragonal and adaptive martensites. We relate this behavior to the frustrated antiferromagnetic coupling between neighboring Mn atoms, which depends on their specific distance and spatial orientation, in particular in martensite.

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Fig. 1: Twin boundary energy γ TB as a function of the twin width specified in lattice planes n of equilibrium non-modulated L10 martensite of Ni₂MnGa (*c/a* = 1.25).



(Abstracts in alphabetical order of the first author's last name; presenting author in bold)

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Synthesis and characterization of perovskite nanoparticles for oxygen evolution catalysis

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Enhancing the large-scale use of electrochemical energy storage and conversion technologies, e.g., for water splitting, requires low-cost, efficient, and robust electrode materials. The development and utilization of non-precious metal-based materials is a promising way to synthesize new catalysts for the oxygen evolution reaction (OER). A specific focus is on metal oxide systems that can be derived from elements that are significantly more abundant than for example the platinum group. One main challenge for these materials systems is to increase the kinetics of the heterogeneous catalytic reactions that are slow due to high overpotentials. Perovskite structures with their high flexibility in composition are promising catalysts and nanoscale, cobalt-based perovskites have recently demonstrated high catalytic activity towards OER [1].

Spray-flame synthesis of high-surface-area nanoparticles allows tuning materials characteristics such as composition, particle size, and morphology over a wide range. The OER activity of sprayflame synthesized LaCoO₃ nanoparticles and the influence of partial substitution of Co by other abundant transition metals have not been studied in detail so far. The motivation of this study is to synthesize and optimize the tailored formation of LaCoO₃ and LaCo_{1-x}Fe_xO₃-based nanoparticles by sprayflame synthesis. Using this technology, we are able to vary the particle size as well as the elemental composition. Perovskite nanoparticles with a size down to 8 nm could be produced. The resulting perovskites were characterized by DLS, TEM, and XPS. Stable dispersions of the materials were processed by spin coating on a glassy-carbon electrode and a variety of electrochemical measurement techniques are applied. Experiments with variable concentration of Fe show that iron is homogeneously incorporated into the LaCoO₃ structure. Interestingly, we identified that residuals of the combustion products partly cover the nanoparticles' surface, which can be removed by heat treatment at 250°C. This annealing step significantly improves the catalytic activity of the nanoparticles for the OER.

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Fig. 1: LaCoO₃ nanopartices doped with 10 at. % Fe by spray flame synthesis and heated at 250°C.

Impact of MOCVD parameters on crystallinity and photoluminescence efficiency in MoS₂ monolayers

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Controlled fabrication of large-area 2D semiconductors is a key technology on the way towards realistic applications of these novel nanomaterials. For upscaling and high productivity, MOCVD systems are most attractive, as they allow for simultaneous growth of 2D materials on a batch of large substrates. MOCVD processes can be tuned for high homogeneity over the wafer, and defined precursor fluxes allow for a precise and reproducible control of growth parameters and composition [1- 4]. The influence of the parameters on nucleation and defect formation is currently under intensive discussion, however, little is known on the resulting impact on photoluminescence (PL) efficiency – an important benchmark for optoelectronic applications.

In our contribution, we use an AIXTRON horizontal hot-wall MOCVD reactor in a 10 x 2 inch configuration for demonstrating routes to reduce defect density and to improve the emission properties of MOCVD MoS₂ monolayers on sapphire substrates [2]. As key parameters to achieve this goal, we identified substrate pre-treatment and variation of the precursor composition. A pre-bake step under N₂ atmosphere prior to growth is found to enhance the PL intensity by a factor of 20, compared with samples grown without pre-treatment or treated under N₂:Di-tert-butyl sulphide (DTBS) atmosphere, respectively, as can be seen in Fig. 1 (top). A complete and homogeneous coverage of the substrate with nanocrystalline MoS₂ monolayers was achieved at T_{growth} = 725 °C with a S:Mo ratio of 476 at a relatively short growth time (2 h). While the small crystal grains (< 25 nm) enable homogeneous coverage, a high defect density obstructs strong PL intensities.

For further quality improvement, we increased the grain size chosing a second set of parameters with T_{growth} = 845 °C and high S:Mo ratio of 175,000. We found a reduced growth rate, resulting in a decreased nucleation density and allowing the formation of crystal grains with sizes of about 75 nm. As demonstrated in Fig. 1 (bottom), the PL linewidth is clearly smaller, indicating a reduced contribution of defect luminescence, and the overall intensity increases by another factor of 3. Corresponding Raman measurements support the PL data: With enlarged grain size, the typical E2g Raman peak of MoS2 becomes spectrally narrower from 4.7 to 3.5 cm-1, confirming a reduced density of defects.

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Fig. 1: Photoluminescence spectra for MOCVD MoS_2 monolayers for different prebake parameters (top) and different crystal sizes (bottom). The insets in the bottom panels are SEM micrographs of the respective structures.

From MAX to MXene – from 3D to 2D

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By now it is well-established that the layered, hexagonal carbides and nitrides with the general formu-Ia, $M_{n+1}AX_n$, (MAX) where n = 1 to 3, M is an early transition metal, A is an A-group (mostly IIIA and IVA) element and X is either C and/or N – sometimes referred to as polycrystalline nanolaminates because every basal plane is a potential deformation or delamination plane - combine some of the best attributes of metals and ceramics. They are excellent conductors of heat and electricity, damage and thermal shock tolerant and fracture toughness values as high as 15 MPa \sqrt{m} . Some are lightweight, stiff and have good creep and outstanding oxidation resistance.(1) More recently we have shown that by simply immersing MAX phase powders, at room temperature, in HF, the A-layers are selectively etched to produce 2D materials that we labeled MXenes to emphasize the loss of the Agroup element and their similarities to graphene. (2, 3) Unlike hydrophobic graphene, MXenes are hydrophilic and behave as "conductive clays", a hitherto unknown combination. MXenes such as Ti₂C, V₂C, Nb₂C and Ti₃C₂, among 20 others (see Fig. 1 for taxonomy) can be used as electrode materials in lithium-ion batteries (LIBs) and supercapacitors (SC), as well as transparent conductive electrodes and EMI shielding, with performances that are quite impressive. In all cases, when used as anodes in LIB, MXenes showed an excellent capability to handle high cycling rates. SC's with volumetric capacitances of > 1400 F/cm³ have been obtained.(4) The potential of using MXenes in energy storage, as transparent conductive electrodes, EMI sheilding among many other applications will be highlighted.

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Fig. 1: Taxonomy of MXenes synthesized to date. Most of these MXenes are derived from their corresponding Al-containing MAX phases. i-MXene refers to in-plane order; o-MXene refers to out of plane order. Over 20 MXene are currently known and dozens theoretically predicted. The vast majority of the work on MXenes has been carried out on the first discovered, $Ti_3C_2T_x$ (1). In this figure the terminations have been ommitted. Adapted from Ref.(5).

Synthesis and cytotoxicity study of spherical boron nitride nanoparticles as potential drug carriers

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Boron nitride nanoparticles are an interesting class of nanomaterials for biomedicine as drug carriers [1-3]. Further, spherically shaped nanoparticles are an important characteristic for large contact area with cell membranes for efficient drug delivery. In the present study, boron nitride (BN) nanoparticles were synthesized by the nebulized spray pyrolysis (NSP) technique. In a typical synthesis, boron trioxide $[B_2O_3]$ and urea $[CO (NH_2)_2]$ were used as precursors mixed in different molar ratios in deionized water. Nitrogen (N_2) was used as a carrier gas. The reactions were carried out by systematically varying the molar ratio, reactor pressure and temperature. The synthesized nanoparticles were characterized by x-ray diffraction (XRD) to analyze the phases formed, Fourier-transform infrared spectroscopy (FTIR) to confirm the bonds, scanning electron microscopy (SEM) and high-resolution transmission electron microscopy (HRTEM) to study the morphology.

The cytotoxicity of a carrier is critical for its application in drug delivery systems. In the present study, MTT assays were done to analyse the cytotoxicity effect of BN nanoparticles in A549 cells. The cells were treated with increasing concentrations of BN from 10 μ g/ml to 150 μ g/ml. MTT assay results showed that concentrations up to 150 μ g/ml did not result in any toxicity to the cells. The results further confirmed that the treatment of A549 cells with boron nitride nanoparticles did not show any remarkable changes in cellular morphology.

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Fig. 1: In vitro cytotoxicity assay. Relative cell viability of A549 cells treated with increasing concentrations of boron nitride nanoparticles.

Synthesis and characterization of titania/tin sulphide (TiO₂/ SnS₂) core-shell nanostructures

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Nanocrystalline semiconductor materials have been progressively gaining in importance in photovoltaic applications due to the large specific surface areas available for light harvesting. In this connection, Titania (TiO₂) nanostructures have attracted a lot of attention, particularly for their stability, efficient charge separation and transport properties. However, their narrow light absorption range, restricted to the UV region makes the efficiency in ambient sunlight relatively low. On the other hand, tin sulphide (SnS_2) nanoparticles have a wider absorption range in the visible regime of the solar spectrum due to their smaller band gap energy [1]. Therefore, functionally graded TiO₂/SnS₂ nano composites are potential candidates in photovoltaic applications with higher efficiency [2].

A simple hydrothermal route was used for synthesizing core-shell TiO₂/SnS₂ nanostructures using titanium isopropoxide and tin chloride as precursors. Characterizations using x-ray diffraction (XRD), high resolution scanning electron microscopy coupled with energy dispersive spectroscopy (HRSEM-EDS) and high resolution transmission electron microscopy (HRTEM) revealed the presence of TiO₂ nano spheres and nanorods in the anatase and rutile polymorph, coated uniformly with nanocrystalline SnS₂ (Fig. 1). Photoluminescence spectroscopy of the synthesized TiO₂/SnS₂ nanostructures showed that the loss of intensity due to recombination in case of the core-shell nanostructure was diminished when compared to pure TiO₂ nanostructures. Further, diffuse reflectance spectra indicated that band gap tuning of the TiO₂/SnS₂ core-shell nanostructure is possible unlike in the case of pure TiO₂ nanostructures.





Fig. 1: HRTEM image of TiO₂/SnS₂ core shell nanostructure

Thermal resistance of twist boundaries in silicon

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In nano-structured thermoelectrics, grain boundaries play an important role in suppressing heat conductance without electrical transport. We present a systematic study of the dependence of the thermal boundary resistance (so-called Kapitza resistance) on the mismatch angle of twist boundaries in silicon [1]. A finite size analysis allows to extrapolate the results for arbitrarily large grain boundary areas A (see Fig. 1). Mismatch angles between 40° and 70° have the largest Kapitza resistance.

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Fig. 1: Non-equilibrium molecular dynamics simulation of heat transport through a grain boundary [1].

Physical vapor deposition of ultrathin magnesium films on H:Si and SiO₂ surfaces: Why does it (not) stick?

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The temperature dependence of magnesium thin film growth on H:Si and SiO2 surfaces is studied by photoelectron spectroscopy. Mg is evaporated from a Knudsen cell onto the substrate at different substrate temperatures between RT and -140°C for both surfaces.

It was found that the existence of a thin SiO2 film on Si reduces the sticking probability for Mg atoms to basically zero at RT, while it is about the same value at 140K for both surfaces. However, upon slowly heating these films created at 140K on SiO2 to RT the Mg film does not desorb but oxidize. Our ongoing experiments are focused to the change in sticking probability with temperature and surface termination [1,2].

The effect may be applied to the preparation of well-defined Mg or MgO nano- and microstructures on Si by local oxidation of the H:Si surface prior to metal deposition.

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Fig. 1: Mg film thickness increase with evaporation time on the H:Si or SiO₂ surface at $T_{\text{substrate}} = \text{RT}$ [3].

Photothermal laser microsintering of nanoporous gold

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Photothermal processing of nanoporous gold using a microfocused continuous-wave laser at a wavelength of 532 nm and a $1/e^2$ spot diameter of 2.9 µm has been studied. In addition, complementary experiments have been carried out via conventional annealing. Scanning electron microscopy has been used for characterization. Local laser irradiation at distinct laser powers and pulse length results in coarsening of the porous gold structures. During laser processing the pore size of the native nanoporous gold increases to maximum values in the range of 0.25 to 3 µm. The affected areas exhibit lateral dimensions in the range of 2-10 µm. Overall two regions are distinguished. An inner region, where large pores and ligaments are formed and an outer region, where the pore size and ligament size gradually change and approach the feature sizes of the native material. A qualitative thermokinetic model allows one to reproduce the experimentally observed dependence of the laser-induced morphologies on the laser parameters. On the basis of this model the underlying processes are attributed to sintering and melting of the gold structures. The presented results demonstrate the prospects of photothermal laser processing in engineering porous gold with spatially varying porosities on micrometer to nanometer length scales, e. g. for applications in catalysis and plasmonics.

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Fig. 1: Laser microsintering of nanoporous Au at varying irradiation time and otherwise constant experimental parameters.

Introducing self-assembled 3D semiconductors

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Organisms have the capability to crystallize shapes with unmatched 3D complexity [1]. Inspired by this, researchers have developed systems to grow complex shapes via coprecipitation of carbonate salts and silica [2]. Such inorganic nanostructured materials with 3D shapes can be of interest for fields such as optics and electronics [3].

In this work we explore this potential by first directing the synthesis of 3D complex shapes such as ones that resemble corals, spirals and vases [Fig 1] [2,4]. Subsequently, we validate the optical properties of these preprogrammed shapes by analyzing the waveguiding through them [4]. These results contribute to our understanding of bioinspired mineralization processes and outline a new nano-fabrication strategy for functional self-organizing materials.

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Fig. 1: Carbonate silica microstructures, scale bar 5μ m, a) SrCO₃ coral, b) BaCO₃ spiral, c) BaCO₃ vases

Single pot synthesis of multicomponent nanoceramics and functional property characterization

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Analogous to high entropy alloys which contain 3 or more metals in nearly-equal proportions [1], multicomponent oxides with more than three principal elements form a new class of ceramic materials [2]– [4]. However, the properties of multicomponent oxides (MCOs) are still being explored and established. In the past studies of MCO systems, isoelectronic cations were chosen on the basis of Hume-Rothery and Pauling's rules. In this study, Fe was doped in the (Co, Cu, Ni, Mg, Zn)O multicomponent transition metal oxide, TMO, system, in order to study the phase formation and the variation in functional properties in the presence of an aliovalent cation.

The system was produced using a single step using a nebulized spray pyrolysis method. (Co, Cu, Ni, Mg, Zn)O formed phase-pure rocksalt structure with the cations in equimolar proportions. The maximum solubility of Fe in the above system was found to 10 mol %, above which a small fraction of spinel phase separated out from the rocksalt lattice. This suggested that increasing the configurational entropy of the system was not the only criteria to stabilize the system as a single phase and that other factors like oxidation state also influenced phase formation. The phase(s) formed and the distortion in the structure were studied using x-ray diffraction (XRD). The product was found to be nanocrystalline from the peak broadening in the XRD pattern and the size of the nanocrystallites was determined using the Scherrer formula. The particle sizes were found to be in the sub-micron range. Functional properties were analyzed using reflectance and fluorescence spectroscopy, I-V measurements, and magnetic studies. The energy band gap (E_{a}) calculated from reflectance and fluorescence spectroscopy data showed that the band gap was in the visible light regime, but the material had an anomalous resistivity, which could be accounted for by the Anderson localization effect [5]. (Co, Cu, Ni, Mg, Zn)O shows paramagnetic behavior up to 5 K, but the addition of 10 mol. % Fe to the system made it ferromagnetic at room temperature. Crystal field theory and interionic exchange interaction could be used to explain this phenomenon.

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Chemical vapor synthesis of hollow β -Fe₂O₃ nanoparticles

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Iron can appear in different oxide phases and valences states. In addition to the well-known α - and γ -polymorphs, β -Fe₂O₃ is another crystalline phase containing iron in the oxidation state of 3+. Since it was first reported in 1956 it has been subject of many studies. Lee et al. reported the synthesis of hollow nanospheres using chemical vapor condensation [1]. They propose a mechanism where the iron(III) acetylacetonate precursor decomposition plays an important role.

Hollow nanoparticles draw interest due to their unique structure and corresponding properties such as low density, high surface area, and distinct optical properties [2]. This enables the manufacturing of advanced materials for example in lithium ion batteries or as gas sensors [3,4].

In this work we study the formation of hollow β -Fe₂O₃ nanoparticles in a hot wall reactor using iron (III) acetylacetonate by chemical vapor synthesis (Figure 1). We propose a Kirkendall type effect of oxidation of intermediate iron metal particles as formation mechanism analogous to the formation hollow ZnO nanoparticles [5]. In order to elucidate the formation mechanism we investigate the change of microstructure and morphology by tuning the supply of oxygen during the synthesis using transmission electron microscopy and X-ray diffraction.

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Fig. 1: TEM image of hollow β -Fe₂O₃ nanoparticles made by Chemical Vapor Synthesis at 800°C.

Nanostructuring 2D Materials by Ion Irradiation

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To fully exploit the colossal technological potential of 2D materials, methods to introduce defects in a controlled way are a key factor. We have investigated energetic ion irradiation induced defects and nanostructures in 2D materials like graphene and single layer MoS₂. We show that apart from the well known binary collisions caused by singly charged keV projectiles, the dense electronic excitation triggered by highly charged ions as well as swift heavy ions may be used to create various characteristic nanostructures each of which may be fabricated by choosing the proper irradiation conditions.

Our experiments, including optical spectroscopy techniques and atomic resolution STEM, reveal unique morphologies such as closed bilayer edges with a given chirality, nanopores of round shape as well as chemical modifications like hydrogenation of the 2D material. By controlled variation of ion parameters like kinetic energy, charge state, angle of incidence, etc., this wide spectrum of modifications in 2D materials can be accessed.

Swift heavy ion nanostructured ultrathin MoS_2 for enhanced catalytic activity

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Nanostructuring the surface of materials in a controlled manner allows significant improvements in fields of electronics [1], membrane technology [2] and catalysis [3]. Large efforts to modify the surface of molybdenum disulfide (MoS_2) in order to increase its suitability for clean energy generation have been devoted in recent years. We follow a novel and faster path: By irradiating two-dimensional molybdenum disulfide by swift heavy ions under grazing incidence, we artificially induce elongated defects along the MoS_2 surface, hence exposing a significant amount of catalytically active side edges. Linear sweep voltammetry measurements show a substantial increase in catalytic activity for the Hydrogen Evolution Reaction as well as a less negative onset potential of irradiated single layer MoS_2 compared to non-irradiated MoS_2 .

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Fig. 1: Schematic of hydrogen evolution reaction at catalytically active sides of MoS₂.

Microstructural manipulation of colloidal films during UV laser sintering

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Nanoparticles as *building blocks* in functional materials require a fine control of the microstructure. Sintering allows the production of microstructures with such desired properties. Among the various sintering techniques laser sintering provides this control due to the short processing time as well as efficient and localized heat deposition [1].

In this work, we present how nanoscaled microstructure of nanoparticulate films – created by colloidal processing (e.g. electrophoretic deposition, inkjet printing) – from nanoparticles obtained by chemical vapor synthesis develop during UV laser sintering. The effect of UV laser processing on the microstructure development is studied by varying the laser parameters (sintering time and laser power). Microstructural characterization of films is performed by X-ray diffraction (XRD) and high-resolution scanning electron microscopy (HRSEM).

Additionally, we report how UV laser sintering is not only suited to manipulate and preserve the nanoscale microstructure but also to synthesize ternary metal oxides of composite films by a new preparation method: reactive laser sintering.

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Fig. 1: Microstructural evolution of nanoparticulate ZnO film at different writing speed.
Magnetic properties of the nanolaminated Mn_2GaC MAX phase

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We study the magnetic properties of a new magnetic Mn_2GaC MAX phase [1]. It is the first synthesized ternary compound with Mn as an exclusive element [2]. The sample is a heteroepitaxial thin film with a naturally formed atomically laminated structure (Fig. 1). Ferromagnetic resonance measurements show an easy axis of magnetization in the film plane [3].

We estimated a magnetocrystalline anisotropy energy density (MAE) of -40 ± 10 kJ/m³. The negative sign indicates that the MAE favors an in-plane direction of the magnetization. Vibrating sample magnetometry (VSM) shows competing ferromagnetic (FM) and antiferromagnetic (AFM) interactions with a saturation magnetization $M_{\rm S}$ = 0.3 µB per Mn atom at T = 100 K (assuming that all spin polarization is located at the Mn atoms). With increasing temperature Mn₂GaC undergoes a first-order magnetic phase transition from a FM to an AFM state at T = 214 K.

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Fig. 1: High Angle Annular Dark Field / Scanning Transmission Electron Microscopy image of a cross section of the atomically layered Mn_2GaC film. The bright (grey) points correspond to Ga (Mn) atomic columns.

Tunable carrier density of two-dimensional hole gases on diamond

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Diamond is a material with promising properties like robustness, high thermal conductivity and high electric breakdown field. Because of the large band gap of $5.45 \ eV$, diamond shows a vanishing intrinsic charge carrier density at room temperature.

On the other hand, surface conductivity induced by a two-dimensional hole gas on the surface, has been demonstrated via hydrogen termination and accumulation of an adsorbate layer [1]. Here, we investigate two-dimensional hole gases (2DHGs) on chemical-vapor-deposition-(CVD)grown diamond after hydrogen plasma treatment and exposure to ambient atmosphere. The 2DHGs are characterized using current-voltage (I-V) measurements and temperature-dependent Hall experiments.

The influence of the surface functionalization, measured by X-ray photoelectron spectroscopy (XPS), on the carrier density and mobility is evaluated.

Hall measurements reveal that the carrier density is increasing from $7.6 \cdot 10^{11} cm^{-2}$ to $1.5 \cdot 10^{13} cm^{-2}$ with increasing amounts of oxygen adsorbed at the surface. In this range, the carrier density remains constant over a temperature range between 4.2 *K* and 320 *K*. For oxygen concentrations above 2.2 % (relative XPS signal), the charge carrier density decreases again and becomes temperature dependent.

This supports a model which includes oxygen-related centers that lead to the transfer of electrons from the surface to the adsorbate layer [2, 3].

The mobility at room temperature increases with decreasing carrier concentration due to the high concentration of impurities in the adsorbate layer. The opposite behavior is observed for 4 K and is attributed to the reduced screening of carriers.

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Fig. 1: Temperature-dependent two dimensional hole mobility for different amounts of adsorbed oxygen (given in percent of relative XPS signal).

Improving the functional properties by stress-induced martensite ageing in ferromagnetic CoNiAl single crystals

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The CoNiAl Heusler alloys can undergo a martensitic transformation to a tetragonal structure (L1₀) from the high temperature cubic B2-austenite and are one of the promising ferromagnetic materials with shape memory effect and high-temperature superelasticity. In the present study, it is shown that stress-induced martensite ageing (the ageing was performed at T = 423 K for 1.0 h under a constant compressive stress of 500 MPa, applied along the [001]_{B2}||[110]_{L10} direction, in the stress-induced martensitic state) is the effective way to improve the functional properties of ferromagnetic Co₃₅Ni₃₅Al₃₀ single crystals. Firstly, stress-induced martensite ageing leads to an increase in the martensitic transformation temperatures on 20-50 K and a decrease in the temperature hysteresis at reversible martensitic transformation during cooling/heating under a compressive load of 150 MPa as compared to the quenched state. Secondly, the necessary condition for the two-way shape memory effect (TWSME) creates by stress-induced martensite ageing of quenched single crystals. It was experimentally shown that the aged crystals demonstrated a good properties of the TWSME response: an operating temperature range (270-320 K), the high cyclic stability of the reversible strain $\varepsilon_{TWSME} = (3.1\pm0.3)$ % during thermal cycles and the low value of the temperature hysteresis ($\Delta T = 24$ K).

This effect of the stress-assisted ageing in the martensitic state is determined the $L1_0$ -martensite stabilization by a diffusion of point defects, which follow in stress-induced martensite symmetry, without precipitation of the dispersed particles [1]. The physical reason for the internal stress field appearance in the stress-induced martensite aged crystals is not fully understood requires further investigation.

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Fig. 1: The strain-temperature response for $Co_{35}Ni_{35}Al_{30}$ single crystals at reversible martensitic B2-L1₀ transformation during cooling/heating: a – under a compressive load of 150 MPa, b – under zero compressive load that demonstrate TWSME.

Magnetic modification and half metallicity of n- and p-type monolayer GaS

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Nanoscience and nanotechnologies have been dominated by two-dimensional (2D) mono-layer materials such as graphene, silicene and germanene. Besides these, group-IIIA metal- monochalcogenides have attracted increasing interest due to their optoelectronic and spin-electronic properties. Achieving the modification of their magnetism is desirable for device applications.[1] In our work, structural, electronic, and magnetic properties of a gallium sulfide (GaS) monolayer with nitrogen(N) or fluorine(F) as a doping atom (see Fig.1.(a)) or as an adsorbed atom (see Fig.1.(b)) are studied systematically using density functional theory (DFT). Our findings show that the pristine monolayer GaS is a non-magnetic, indirect bandgap semiconductor. Magnetization with local magnetic moment of 1.0µB can be induced through N atom doping at the S-site. The material can become a direct bandgap semiconductor (nonmagnetic) upon N atom doping at the Ga-site. Similarly, by adsorption of N on top of S (TS) or on top of Ga (TGa) the magnetic moments are 1.0µB and 3.0µB, respectively. A semiconductor-to-metal transition occurs upon F doping at the S-site. Similarly, F doping at the Ga-site, adsorption at the TS and the TGa site have magnetic moments of 0.11µB, 1.0µB and 1.0µB, respectively. Half-metallic behaviour is studied in case of N, F adsorption at the TS site and F adsorption at the TGa site. The indirect band gap of the pristine GaS monolayer is rendered direct in one spin channel by introducing N at S-site and TS, and F adsorption at TS. These results suggest that GaS could be made ferromagnetic by doping or adsorption and thus is a good candidate for design and construction of 2D optoelectronics and spintronics devices.

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Fig.1: Top view of the monolayer β -GaS 4×4×1 supercell, with substitutional dopant sites at a Ga atom, a S atom, on top of a S atom (TS) and on top of a Ga atom (TGa). The dashed line represents the unit cell within the supercell (a) Side view of the same supercell to indicate adsorption for N and F at TS and TGa, h represents the S-S distance, bGa-Ga denotes the Ga-Ga bond length, bGa-N M denotes the adsorption bond length for N(F) at TGa, bS-N M denotes adsorption bond length for N(F) at TS. Light yellow spheres indicates S atoms and purple spheres indicate Ga atoms. Red sphere indicate F atoms and black sphere indicate N atoms.

Edge pinning effects in electromigration

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By means of Kinetic Monte Carlo simulations the mechanisms are analyzed by which impurities slow down electromigration. The effect of a single Cu-atom embedded in the surface of a Ag-wire is considered. It is shown that island edges get pinned, and that the depinning by thermal fluctuations determines the resulting electromigration velocity [1]. In the case of migrating monolayer holes in the Ag-surface the pinning mechanisms are different. They depend on the size of the hole and on the position of the impurity in the uppermost or in the second atomic layer.

[1] M. Jongmanns, A. Latz, D.E. Wolf, Europhysics Letters 110 (2015) 16001



Fig. 1: Silver island with a copper impurity (green) electromigrating on a silver surface. Current direction is from right to left. Between times t_1 and t_2 the island is pinned.

Gas and humidity sensors made from Ti₃C₂ MXene

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Two-dimensional materials are of great interest for application and basic sciences due to their sometimes very special properties, like linear dispersion relation in Graphene. We have investigated the conductivity of a clay made of Ti₃C₂ MXenes [1], which were in a first step produced as volume like material. Using an etching process, two-dimensional flakes were produced. The influence of the surface termination of these flakes was than investigated by measuring the resistivity after oxygen and hydrogen plasma treatment in situ. We were able to reduce the resistivity by 20% from the oxidized to the reduced state (Fig. 1). In addition we found out, that these structrues are excellent humidity sensor. They change their conductivity by a factor of 26 when increasing the relative humidity from 0% to 80%.



[2] M. Ghidiu et al. Chem. Mater. 28 (2016) 3507–3514, DOI: 10.1021/acs.chemmater.6b01275



Fig. 1: Resistivity vs. total time of plasma treatment of a clay made of MXene. The resistivity can be controlled from 5.6 $\mu\Omega m$ (oxidized state) to 4.6 $\mu\Omega m$ (reduced state) by plasma treatment.

Fe-microwalls in permalloy by laser beam melting induced segregation

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The soft magnetic material permalloy (Fe20wt.-%Ni80wt.-%) and related Fe-Ni-alloys exhibit remarkable electrical and magnetic properties [1,2]. Due to their high permeability, low coercivity and high magneto-conductivity in weak magnetic fields they are used in a wide range of applications such as transformers, sensors, inductive devices and electric motors [3-5]. However, conventional powder metallurgy methods have several drawbacks including a decrease of magnetic properties [6], geometry limitations, non-net-shape parts and accordingly higher costs due to post-treatment.

Additive Manufacturing (3D printing) offers an interesting approach. In Laser Beam Melting (LBM) material is added successively (layer wise) to build up the shape of a body. The most striking advantage of LBM is the possibility to create individualized net shaped structures and complex geometries in a single step directly from a CAD model, which is impossible to realize with other processes [7].

We report the additive manufacturing of Fe-Ni magnets with the composition of 20 wt.-% Fe and 80 wt.-% Ni by laser beam melting.

Separate Fe and Ni powders with a particle size distribution between 10 and 45 µm were mixed and cubes with an edge length of 5 mm were produced. For high energy input (high laser power and low scanning velocity) Energy-dispersive X-ray spectroscopy revealed the segregation of Fe and Ni at the surface of the cubes. Figure 1 shows the surface consisting of two phases, a nickel-rich FeNi-phase and wall-like microstructures consisting of almost pure Fe.

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Fig. 1: EDX-mapping of Laser Beam melted powder mixture with the composition of 20 wt.-% Fe and 80 wt.-% Ni. Fe:Blue , Ni:Green, O:Yellow.

Catalyst free growth of ZnO nanorods by chemical vapor deposition

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Zinc oxide (ZnO) is a semi-conductor with a large band gap of 3,37 eV [1], hence it has huge potential for application in electronics and optoelectronics. Moreover, ZnO presents minimal health hazard when compared with other semi-conductors and can be used for medical purposes [2], such as in vivo detection of cancer cells, a consequence of their optical properties and biological degradability [3]. ZnO nanorods have various useful properties due to their one-dimensional structure and high aspect ratio. For example, these nanorods can be used as piezo electric field effect transistors and thus as force sensors [4].

We have successfully synthesized ZnO nanorods on Si-substrates coated with a ZnO seed layer in a tube furnace by a mixture of pure zinc (Zn) vapor, argon (Ar) and oxygen (O2) at 650°C using chemical vapor deposition (CVD). Unlike conventional methods such as vapor-liquid-solid (VLS) growth, this approach is more economical, due to lower process temperatures and absence of metal catalysts during synthesis. By varying time of synthesis we have obtained nanorods with various lengths and diameters. Also, it was observed that the dispersion of the rods depends on the density of the ZnO seed layer at substrate surface. X-ray diffraction (XRD) measurements show that the ZnO nanorod samples are of wurtzite crystal structure. The diversity of the crystal growth morphology of the ZnO structures, caused by varying process parameters, was investigated by employing scanning electron microscopy (SEM).

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Fig. 1: SEM Image of hexagonal ZnO nanorods grown at 650°C on silicon without a metal catalyst



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