Brandenburg
University of Technology
Cottbus - Senftenberg

Call for Applications – 6 Ph.D. Scholarships

Thematic Cluster "Functional Materials and Film Systems for Efficient Energy Conversion (FuSion)"

of the BTU Graduate Research School

The Brandenburg University of Technology Cottbus-Senftenberg will launch new thematic clusters in the Graduate Research School (GRS) as part of the strategy to strengthen the research profile of BTU. Thematic clusters are flexible units that shall contribute to the creation of critical masses in the core research areas of BTU. At the same time they are an important instrument of promoting young researchers.

Against this backdrop the BTU will establish in October 2016 the thematic cluster *"Functional Materials and Film Systems for Efficient Energy Conversion (FuSion)"*. Successful applicants are expected to begin their research in October 2016 and the scholarship will be tenable for 36 months. The amount of the scholarship is 1,400 € / month. For some of the positions cooperating institutes will provide a topping-up amount. The GRS will also offer child support for Ph.D. students with children. Successful candidates will have access to additional funding of the GRS for their doctoral research (e.g. mobility grants etc.).

<u>Description of the cluster:</u>

Energy efficient sensing and computing requires novel technologies and approaches for virtually every component of smart sensors. This comprises system and processor architecture, sensing and computing algorithms, batteries and energy harvesting as well as energy conversion.

The Graduate Research School Cluster "Functional Materials and Film Systems for Efficient Energy Conversion (FuSion)" aggregates and focuses research activities at BTU Cottbus-Senftenberg and the non-university research organizations Leibniz IHP, Frankfurt Oder, Leibniz IKZ, Berlin and Fraunhofer IPMS, Dresden with the objective to gain a deeper, interdisciplinary-based understanding of materials, processes and film systems supporting novel approaches and solutions for efficient energy conversion. The program offers six individual, up-to-date research topics within this field. These research topics, each to be investigated by one doctoral student and supported by several senior scientists of various disciplines, are assigned as follows:

- **Materials** for energy storage and energy efficient computing, 2 individual topics
- **Processes** for energy harvesting devices, 2 individual topics
- Thin Films and **Film Systems** for energy efficient transducers, batteries and catalytic applications, 2 individual topics

Within each individual project several experimental methods ranging from layer deposition to material characterization as well as theoretical and modeling methods will be applied. Close interaction of the scientific participants, with access to the infrastructure of the university as well as of the non-university research institutes, and with a wide range of expertise of the senior scientists provides an excellent basis for the research activities and in particular for the qualification of each doctoral student.

<u>Requirements:</u>

Successfully or nearly finished master or diploma degree graduates in natural science or applied science with excellent grades and a strong interest in conducting research from an interdisciplinary perspective are encouraged to apply. In addition,

- candidates are expected to show high readiness for teamwork within the cluster and,
- applicants should be able to work autonomous in a high quality way.

<u>Working language:</u> German/English

<u>Language of dissertation:</u> German/English

<u>Required documents:</u>

For evaluation a meaningful application including covering letter with a statement of research interest and experience regarding one of the six topics, CV, master/diploma certificates with transcript of records, at least one reference letter, a summary of the completed master/diploma thesis and if applicable the most relevant publication should be provided most useful in digital form.

<u>Gains:</u>

FuSion PhD-candidates benefit from:

- Internationally and interdisciplinary focused PhD program
- Cooperation with renowned non-university institutions
- Regular thesis discussions with peers and supervisory teams
- Accompanying cluster workshops with excursions to the facilities of the participating working groups
- Winter/summer schools at participating partners
- Courses on personal skills, networking, scientific techniques and scientific writing, as well as on generic competences and soft skills

Application:

Please note that the cluster only accepts complete applications. The application deadline is October 4, 2016. Please send your application (preferably via e-mail as one PDF) to the respective person mentioned in the individual scholarship.

For further information please contact:

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Research topic Materials 1
Academic supervisor
Prof. Dr. rer. nat. habil. Götz Seibold
Doctoral thesis
Plasmonic excitations in graphene with periodically modulated superstructure
Description and objectives
Plasmonics based on graphene is a current hot topic in solid state physics and deals with the excitation, manipulation and utilization of surface plasmon polaritons, i.e. quasiparticles arising from the coupling between electronic collective motion and light. In graphene these excitations are in the terahertz to mid-infrared regime which suggests a variety of applications in information and communication, chemical and biological sensing, spectroscopy etc. The realization of THz-information and communication technologies would be of great importance in connection with efficient energy conversion since it enables high-performance wireless connections without any losses which would occur in wired networks. Tunability of the plasmon excitation can be achieved by either changing the carrier concentration (i.e. the chemical potential) of by creating so-called plasmonic nanostructures which allows for tailoring the electromagnetic response to a particular region of the electromagnetic spectrum, especially the “terahertz gap”. Within the PhD project it is planned to study the plasmon excitations within the random phase approximation based on a tight-binding model of graphene supplemented with a periodic modulation of the chemical potential. In particular, we are interested in the change of the plasmon frequency by changing the amplitude, structure, and periodicity of the modulation which then has strong implications for the tuning of graphene as a plasmonic metamaterial. In addition to the microscopic approach it is also planned to study the plasmon structure on a more intuitive level by applying a hybridization model developed for the description of the plasmon response of complex nanostructures (E. Prodan et al., Science 302, 419 (2003)). The combination of both microscopic and qualitative description will then allow for a coherent view of the plasmon dynamics in electronically modulated graphene material.
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Research topic Material 2
Academic supervisor
Prof. Dr. rer. nat. habil. Olaf Klepel
Doctoral thesis
Development of porous surface functionalized carbon materials for electrochemical and catalytic applications
Description and objectives
Porous carbons are used as adsorbents, catalyst supports in heterogeneous catalysis as well as electrode materials. Currently, additional fields of application such as the use as a storage medium for hydrogen or the use in electrochemical applications for energy conversion and energy storage is becoming increasingly important. Carbon electrodes are for example a component of fuel cells, lithium ion batteries and electrochemical double layer capacitors. Despite the wide variety of (potential) applications, the key selection criteria of carbon materials can be traced back to relatively few characteristics: pore-size distribution, chemical composition, the proportion of graphitic structures or particle design. Therefore, processes for customised production of carbon materials in consideration of these factors have long represented a challenge. A modular concept would be desirable which allows the customized preparation of porous carbon materials ideally by variation of one of the above-mentioned parameters while keeping the other parameters constant. A current doctoral thesis of the group therefore focuses on the development of a library of carbon-based catalysts, which are systematically modified in regard to degree of graphitization and the content at the impurity atom nitrogen. The influence of electronic (and thus catalytic and electrochemical) properties of the carbon material) is attributed to nitrogen atoms. In the PhD-thesis, the range of modifying heteroatoms shall be extended by, for example, sulphur and phosphorus. Here, the challenge is to eliminate the effects of impurities on other material properties (pore-size distribution and structure) as far as possible in order to come close to realizing the above-mentioned concept of a modular synthesis. The developed materials should be tested - in cooperation with other working groups - particularly in electrochemical applications (batteries, capacitors).
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Research topic Processes 1
Academic supervisor
Prof. Dr. rer. nat. habil. Jörg Acker
Doctoral thesis
Chemical reactivity of disturbed silicon surfaces
Description and objectives
Lattice defects and mechanical stress conditions, plastic deformation, modification due to phase transitions and local contaminations, which not only affect the surface but also reach into the solid for several micrometers, exert an enormous influence on the chemical reaction behaviour. Such disturbed surfaces exhibit unusual reaction behaviours which manifests itself in higher reaction rates or unexpected reaction processes. Wire-sawn silicon wafers from solar cell production serve as a model system for such disturbed surfaces. In the production of solar cells, this damage zone is removed by etching processes whereby a specific topography, the so-called texture, is simultaneously imprinted on the surface. Influencing the degree of reflectance the texture of the surface makes an important contribution to the efficiency of a solar cell. However, it is yet widely unknown how the nature of the imperfections within the surface damage affects the chemical reactivity of silicon, likewise in the process of wet-chemical etching. This doctoral research project is focused on the study of the basic relationships how the types of imperfections on silicon surfaces as well their extent affect or alter the chemical reactivity compared to monocrystalline silicon by means of microscopic methods, such as confocal Raman microscopy, electron microscopy and laser confocal microscopy. This goal consists of three main challenges: • The first is the preparation and characterization of imperfect surfaces by confocal Raman spectroscopy, electron microscopy and laser confocal microscopy. Imperfections into monocrystalline silicon can be introduced by scratches, fractures, high-pressure modifications of Si, mechanically induced lattice strain, or alloying. Additionally, solar wafer with surface damage have to be studied. • The second is the study the reactivity of imperfect silicon surface in terms of reaction kinetics, description of the chemical processes, and shaping the topography of the surface by means of suitable model reactions systems which have to be tested and selected before. • The third is to understand and to model the obtained results quantitatively.
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Research topic Processes 2	
Academic supervisors	
Prof. Dr. rer. nat. habil. Peer Schmidt / Dr. Torsten Boeck	
Doctoral thesis	
MBE growth of Si, Ge and SiGe nanowires and modeling of synthesis conditions for multi-component compounds for thermoelectrics	
Description and objectives	
The use of SiGe nanowires for thermoelectric devices is a promising and interesting research area because, in addition to very good thermoelectric properties, the effect of phonon scattering on the surfaces of nanostructures can be utilized. The topic combines fundamental and theoretical questions of materials research with applied and experimental aspects of modern crystal growth. According to the current state of literature, the thermoelectric efficiency of SiGe alloys is at its highest amount at a Ge content of 30 % to 40 %. The growth of large volume crystals of good quality in this concentration range has not been successful due to the wide miscibility gap with the established procedures of solid crystal growth. It would also be too expensive for industrial use. An alternative is the growth of nanowires as carried out at the Leibniz Institute for Crystal Growth (IKZ) by molecular beam epitaxy (MBE) using the vapor-liquid-solid mechanism (VLS). One focus of the planned thesis about the growth of Si, Ge or SixGe1−x nanowires is the qualitatively and optionally quantitatively investigation of the influence of the chemical or physical quantities (i) Si/Ge composition, (ii) supersaturation of the metal catalyst and (iii) surface energy of the growing nanowires in order to specifically influence the direction of growth as well as the faceting. Although the nanowire growth generally occurs along the direction with the lowest free energy, it was revealed that Si and Ge nanowires grow in different directions under otherwise identical test conditions. However, growth direction and faceting are fundamental questions for the use of nanowires in future devices. An uniform growth perpendicular to the substrate would be desired, preferably on Si(111) substrates. It is also important to establish defined doping. A concept should be realized enabling the production of p- and n-doped nanowires on substrates, which are separate at first. Then the nanowires have to be interconnected to a series of thermal elements, where the legs of a thermocouple consists of an ensemble of p- and n-doped nanowires each. In addition to the characterization of the structures by SEM, TEM, AMF, X-ray and electrical methods, the modeling of the growth and special physical effects plays an important role. By using thermodynamic modeling (CalPhaD method: programs FactSage, TRAGMIN) the state systems involved in crystallization (solid-liquid, solid/liquid-gas) should be detected and the reaction paths during the deposition of the crystals should be simulated. It is of particular interest under which experimental conditions a targeted deposition of phases with defined quantity parameters Si/Ge is possible.	
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Research topic Film Systems 1
Academic supervisor
Prof. Dr.-Ing. Dr. rer. nat. habil. Harald Schenk
Doctoral thesis
Studies and optimization of thin film layer properties in high efficient electrostatic actuators
Description and objectives
Energy efficient operation of transducers is of increasing importance in particular in the context of the strongly emerging Internet of Things and the increasing number of mobile and wearable devices in consumer electronics. Miniaturized transducers for e. g. motion detection, sound generation or on-site analytical tasks with low energy consumption are required to stay within the limits of available power resources. Due to scaling effects and the straight-forward integration into high volume fabrication processes, transducers based on electrostatic effects for sensing and actuation are of high interest, currently and in the future. Together with the Fraunhofer IPMS, BTU CS demonstrated a novel, high efficient electrostatic actuator principle to be integrated into various MEMS sensors and actuator systems. The PhD-thesis will focus on integration of the novel principle into a CMOS-compatible process. Hereby, investigation of material properties taking into account high electrical and mechanical loads is of particular interest. The influence of various dielectric and metal layer materials, interfaces and their quality including stoichiometric aspects on parasitic dielectric charging as well as on electrical and mechanical degradation in operation has to be studied in detail. In close consultation with process engineers of Fraunhofer IPMS' cleanroom facilities, suitable combinations of layer materials and deposition and patterning process conditions have to be selected and characterized by means of test devices, applying C-V and I-V measurement methods, as well by means of various micro- and nanoscopic material characterization methods. Based on the findings of these and further characterization results complete functional actuator layers will be devised, fabricated and characterized. A further objective is to correlate the observed effects of the actuators with the characterization results of single layers and layer stacks and to develop a semi-quantitative physical model to describe respectively predict failure phenomena. Thereby, the final goal is to develop approaches towards highly reliable device operation.
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Research topic Film Systems 2
Academic supervisor
Prof. Dr. rer. nat. habil. Dieter Schmeißer
Doctoral thesis
Thin and conformal ALD deposited Co and Ni metal layers for battery and catalytic applications
Description and objectives
The goal of the thesis will be the investigation and development of atomic layer deposition (ALD) of thin Cobalt (Co) and Nickel (Ni) layers. Here two directions should be followed. On the one hand, on the basis of thermal ALD, the development should be established by the deposition of pure (NiO, CoO) and ternary oxide layers (CoNiO) and their subsequent reduction. In contrast, plasma enhanced ALD (PEALD) will be used to follow a direct route of metal deposition, where plasma radicals (oxygen, hydrogen, nitrogen) will be used to fulfill reductive conditions where thermal activation is not sufficient. Metal-organic precursors will be used with special focus on their complex properties and technical manageability. The deposited layers will be characterized by spectroscopic and microscopic methods to determine the layer composition, morphology, and homogeneity. Further essential criteria will be the conductivity of the layers. The advantages and disadvantages between thermal ALD and PEALD have to be worked out and weighted for potential applications. Thin and conformal Co and Ni metal layers are of interest for the CMOS technology (silicide formation for small contact resistances, adhesion layer for interconnects), for magnetic and nano-crystalline non-volatile memories and in particular for catalytic applications. In addition, ternary Co/Ni oxides are used in lithium-ion batteries; here the Co/Ni ratio might be controlled very effectively by ALD. In many applications, the conformal growth on 3D structures is important for the efficiency and life-time of the devices. The conformity of the layers depends strongly on the deposition method; here the ALD is favorable due to the extremely precise thickness control in comparison to other techniques (CVD, PVD). Hence, the topic has a direct link to energy conversion on the one hand (batteries, catalysts for photo-catalytic water splitting); on the other hand ALD layers can contribute to performance improvements and therefore to higher energy efficiency.
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