HL 92: Poster Session: Structure and transport in organic photovoltaics; Photovoltaics; Impurities/Amorphous semiconductors; New materials

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Thursday 16:00–20:00 Location: Poster A

HL 92.1 Thu 16:00 Poster A

Nanostructured metal oxides for hybrid solar cells — •Julian Reindl[1], Jonas Weickert[1], Andreas Wisnet[2], Sophia Betzler[2], Christina Scheu[2], and Lukas Schmidt-Mende[1] — [1]Hybrid Nanostructures, FB Physik, Universität Konstanz — [2]Department of Chemistry and Center for Nanoscience, LMU München

Organic solar cells are an interesting technology to realize low-cost photovoltaics on a large scale. Even though efficiencies beyond 8 % have been achieved with a mixed film of donor and acceptor for thin films of about 100 nm, the unordered inner morphology of the active layer has detrimental effects in thicker layers due to more pronounced charge trapping and charge carrier recombination. A promising approach to realize thicker active layers with accordingly higher absorptivity is the hybrid solar cell concept, where the organic donor is substituted by a wide band gap metal oxide like titania (TiO2). Due to the small exciton diffusion length in organic semiconductors of usually 10-20 nm a structured donor-acceptor interface with this dimension is supposed to support efficient exciton separation and therefore lead to decreased recombination in these devices.

Here we present different approaches of fabricating a structured hybrid solar cell where we use either structured TiO2 wires with controllable dimensions or a structured transparent electrode underneath a thin TiO2 layer. The first attempt provides a crystalline acceptor matrix whereas the latter takes advantage of short pathways for electrons from the donor-acceptor interface to the collecting electrode.

HL 92.2 Thu 16:00 Poster A

Morphology and interdiffusion in organic donor-acceptor blends studied by analytical TEM — •Diana Nanova[1,2,4], Dominik Daume[2,4], Levin Dieterle[1,3,4], Martin Pfannmöller[3,4], Rasmus R. Schröder[3,4], and Wolfgang Kowalsky[1,4] — [1]Institute for High-Frequency Technology, TU Braunschweig, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [3]CellNetworks, BioQuant, Heidelberg University, Germany — [4]InnovationLab GmbH, Heidelberg, Germany

We present a combined study of the morphology and its relation to function on model devices of organic solar cells. The device characteristics acquired from impedance spectroscopy are correlated with the microstructural properties, obtained from analytical TEM. We found a novel morphology of P3HT:PCBM by applying electron energy loss spectroscopy and electron spectroscopic imaging in the low energy loss region. We observed a mixed-phase at the interface between the PCBM-rich and P3HT-rich phase, which seems to be crucial for efficient charge separation. To study the phase separation kinetics at the donor-acceptor interface, planar heterojunction samples of P3HT/PCBM bi-layer assemblies were prepared and annealed at various temperatures. In order to investigate the formation of a composite phase at the bi-layer interface via TEM, we prepared cross-sections by different methods, e.g. FIB-milling. We observed a change in the interface structure due to recrystallization and interdiffusion during annealing. This process leads to changes in the capacitance of the bi-layer devices, which can be derived from the measured impedance spectra.

HL 92.3 Thu 16:00 Poster A

Scanning Kelvin Probe Microscopy on FIB-milled crosssections of different organic photovoltaic devices — •Christian Müller[1,2,3], Rebecca Saive[1,2,3], Michael Scherer[1,2,3], Michael Kröger[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institut für Physik, University Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

Scanning Kelvin Probe Microscopy (SKPM) is a powerful tool to investigate the charge transport in organic devices and has been successfully applied to Organic Field Effect Transistors (OFETs). Conventional SKPM is restricted to the device's surface. Hence we have developed a new method to investigate device's cross-sections by milling with a Focused Ion Beam (FIB) and adjacent Scanning Probe Microscopy (SPM) characterization. We applied this method to organic solar cells and could reveal the potential distribution along the charge transport path. Sample preparation and measurements were performed in-situ in a combined SEM/FIB crossbeam system with an integrated SPM to avoid sample degradation by ambient air.

HL 92.4 Thu 16:00 Poster A

Influence of intercalation on geminate and nongeminate recombination in organic bulk heterojunction solar cells — •Benedikt Allendorf[1], Andreas Zusan[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The fundamental understanding of charge carrier generation and recombination is one of the key issues for further optimization of organic photovoltaics. Generation of free charge carriers with a high yield is a crucial step to ensure high power conversion efficiencies. We study how it is influenced by the morphology of the photoactive layer. We processed organic bulk heterojunction solar cells from blends of poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT) with different fullerene acceptors. The blend of PBTTT donor with phenyl-C71-butyric acid methyl ester ($PC_{71}BM$) leads to intercalation of the acceptor molecules between the side chains of the conjugated polymers. In contrast, the bisadduct of phenyl-C61-butyric acid methyl ester (bis-$PC_{61}BM$) as acceptor material does not intercalate due to its larger volume. By means of time delayed collection field (TDCF) measurements we gain insight into the field dependence of polaron pair dissociation as well as into nongeminate recombination. Finally, we discuss the influence of intercalating and non–intercalating acceptors on generation and recombination of free charge carriers in organic solar cells.

HL 92.5 Thu 16:00 Poster A

Modeling disordered morphologies in organic semiconductors — •Tobias Neumann[1], Denis Danilov[1], Christian Lennartz[2], and Wolfgang Wenzel[1] — [1]KIT Campus Nord Gebäude 640 D-76344 Eggenstein-Leopoldshafen — [2]BASF Ludwigshafen

Organic thin film devices are investigated for many diverse applications, including light emitting diodes, organic photovoltaics and organic field effect transistors. Modeling of their properties on the basis of their detailed molecular structure requires generation of representative morphologies for these systems, many of which are amorphous. Because time-scales for the creation of morphologies are slow, we have investigated a linear-scaling single-molecule deposition protocol which generates disordered morphologies in a protocol that emulates vapor deposition of molecular films. Here we have applied this protocol on 5 test systems, with and without post-processing of the individually deposited molecules at every step. For the two simple systems, a noble gas and buckminster fullerenes, we managed to deposit ordered structures. Furthermore we investigated the properties of amorphous structure of films made of Alq3, PCBM and Alpha-NPD molecules, which are widely used in organic electronics, and compared our results to molecular dynamics simulations for each molecule.

HL 92.6 Thu 16:00 Poster A

Texturization and Passivation of Monocrystalline Silicon Wafers for High-Efficiency Solar Cells — •Jan Kegel[1,2], Mathias Mews[2], Heike Angermann[2], Uta Stürzebecher[3], and Bert Stegemann[1] — [1]Hochschule für Technik und Wirtschaft, Berlin, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Erfurt, Germany

Wet-chemical treatment of crystalline Si wafers for the preparation of heterojunction solar cells are optimized with respect to low reflection losses, low recombination losses and long carrier lifetimes. It is demonstrated that a joint optimization of both saw damage etch and texture etch is necessary to control the optical and electronic proper-

ties of the resulting pyramid morphology. Effective surface passivation is achieved by deposition of intrinsic amorphous Si (a-Si:H(i)) layers. We demonstrate that optimized parameters for deposition of a-Si:H(i) on planar wafers can be transferred to the deposition on textured substrates. Moreover, the influence of the deposition temperature on the optical layer properties is elucidated, and the impact of post-deposition plasma-hydrogenation and annealing on the charge carrier lifetime and the implied open-circuit voltage is revealed.

HL 92.7 Thu 16:00 Poster A

Investigating the infrared conversion efficiency of Black Silicon solar cells by measuring the differential spectral responsivity (DSR) — •Kay-Michael Günther[1], Stefan Winter[2], Thomas Gimpel[3], Wolfgang Schade[1,3], and Stefan Kontermann[3] — [1]Clausthal University of Technology, EFZN, Am Stollen 19B, 38640 Goslar, Germany — [2]PTB Braunschweig, Bundesallee 100, 38116 Braunschweig, Germany — [3]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

Exposing a silicon surface to femtosecond-laser pulses under a SF6 atmosphere leads to the incorporation of sulfur, which acts as a donor. After several pulses on the same spot, the surface becomes roughened. Therefore, with a single fabrication step, a pn-junction as well as a low reflecting surface can be created. This material is called Black Silicon. Previous works showed, that Black Silicon has a very high absorptance in the infrared region. It is believed, that high concentrations of sulfur states lead to the formation of an intraband within the bandgap.

To investigate the conversion efficiency of a Black Silicon Solar cell in the infrared, we measure the differential spectral responsivity in the range from 280 to 1200 nm. Compared to a standard high efficiency silicon solar cell, the Black Silicon cell of the same size exhibits a significantly increasing spectral responsivity above 1030 nm and even a higher spectral responsivity above 1150 nm.

HL 92.8 Thu 16:00 Poster A

Investigation of the sulfur doping profile of femtosecond-laserdoped Black Silicon solar cells — •Kay-Michael Günther[1], Alexander Bomm[2], Thomas Gimpel[2], Michal Schulz[1], Holger Fritze[1], Wolfgang Schade[1,2], and Stefan Kontermann[2] — [1]Clausthal University of Technology, EFZN, Am Stollen 19B, 38640 Goslar, Germany — [2]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

Irradiating silicon with femtosecond-laser pulses under a SF6 atmosphere leads to the incorporation of sulfur and a structured surface. Very high sulfur concentrations can be achieved and an enhanced absorptance in the infrared spectral region is observed. This material is called Black Silicon and is used to fabricate solar cells and infrared photodetectors.

In this work, we investigate the sulfur doping profile of Black Silicon with 5 pulses per spot with secondary ion mass spectroscopy (SIMS) and capacitance-voltage spectroscopy (CV). Due to the strong surface roughness and the intrinsic pn-junction of the material, we applied a CV technique which uses impedance spectroscopy (IS) to compensate for additional space charges and series resistances. We compare samples with different annealing steps and different process atmospheres and we show that only a part of the incorporated sulfur is electrically active.

HL 92.9 Thu 16:00 Poster A

Optimization of indium tin oxide-free semitransparent polymer-based solar cells — •Verena Wilkens[1], Antonio España Petatañ[1], Sebastian Wilken[1], Kambulakwao Chakanga[2], Omid Madani Ghahfarokhi[2], Karsten von Maydell[2], Jürgen Parisi[1], and Holger Borchert[1] — [1]University of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany — [2]Next Energy, EWE-Forschungszentrum für Energietechnologie e.V., 26129 Oldenburg, Germany

The absorption of conjugated polymers is usually limited to the visible range, which leads to lower photocurrents of polymer-based organic solar cells (OSCs), compared to established technologies based on inorganic semiconductors. On the other hand, such narrow absorption profiles enable the realization of semitransparent devices, which can be utilized in power-generating window applications. The most challenging issue for that purpose is the development of almost transparent contacts with sufficient electrical properties. Here, we present semitransparent OSCs based on poly(3-hexylthiophene) (P3HT) and phenyl-C_{61}-butyric acid methyl ester (PCBM), which are free from the expensive transparent conductor indium tin oxide (ITO). Instead of ITO, we report on the application of aluminum-doped zinc oxide (ZnO:Al), prepared by dc-magnetron sputtering. As hole contact, ultra-thin films (e.g. Ag or Au) with an adequate transparency in the required wavelength regime were used. We introduced additional interfacial layers like molybdenum oxide (MoO_3) and tungsten oxide (WO_3), in order to improve charge extraction and light incoupling.

HL 92.10 Thu 16:00 Poster A

Application of $CuInS_2$ and ZnO nanoparticles in colloidal quantum dot photovoltaics — •Dorothea Scheunemann, Sebastian Wilken, Katja Frevert, Florian Witt, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

Colloidal quantum dots (CQD) are attractive for photovoltaics because of their solution processability and spectral tunability due to quantum size effects. Rapid advances in CQD photovoltaics in the recent years have led to high power conversion efficiencies. Previous works mainly focused on highly toxic materials containing cadmium or lead which might limit their possible application. One promising alternative material is $CuInS_2$ (CIS) which has shown attractive device performance in thin film solar cells. Here, we present solution processed CIS nanoparticles as absorber layer in nanocrystal based solar cells. In order to achieve efficient charge separation we use a heterojunction based on a bilayer structure of CIS and intrinsically n-doped ZnO nanocrystals. One issue in thin film photovoltaics is the optimization of the absorber thickness, taking into account light absorption as well as charge carrier collection. Therefore, we determined the absorption coefficient and transport properties which can serve as input parameters into an electro-optical simulation in order to determine the optimal absorber thickness.

HL 92.11 Thu 16:00 Poster A

Investigation of stacked elemental layers for Cu(In,Ga)Se_2 thin film preparation by rapid thermal selenization — •Christiane Stroth, Jörg Ohland, Ulf Mikolajczak, Thomas Madena, Jan Keller, Jürgen Parisi, Maria Hammer, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Rapid thermal selenization of pure metallic (Cu-In-Ga) or selenium-containing (Cu-In-Ga-Se) precursors is a favorable method to fabricate Cu(In,Ga)Se_2 absorber films for application in thin film solar cells. Because of its upscaling potential and the short process time it is a promising approach for the fabrication of CIGSe photovoltaic modules on industrial scale.

As a preliminary work for prospective plasma-enhanced selenization of stacked elemental layers (SEL) the elements copper, indium and gallium were sequentially deposited on molybdenum coated soda-lime glass by thermal evaporation. The stacking order was varied and the precursors were annealed with different heating rates. Morphology, elemental depth distribution and phases of the layers were investigated before and after annealing using scanning electron microscopy, energy-dispersive X-ray spectroscopy and X-ray diffraction. Furthermore the influence of different heating rates on phase transitions during annealing was studied by in-situ X-ray diffraction.

HL 92.12 Thu 16:00 Poster A

Temperature-dependent quantum efficiency measurements on Cu(In,Ga)Se_2 thin film solar cells — •Thorsten Sonnet, Janet Neerken, Dirk Otteken, Jürgen Parisi, Ingo Riedel, and Maria Hammer — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Solar cells based on Cu(In,Ga)Se_2 absorber layers demonstrate high power conversion efficiencies around 20%. However, solar cells obtained from industrial production exhibit lower efficiencies. In order to understand the physical mechanisms, the characterization of internal and external losses of the solar cell is important. While the temperature dependence of the open circuit voltage of the cells is an established tool to characterize recombination processes, the fact of a temperature dependent photocurrent is often overlooked. In order to characterize the collection efficiency, temperature-dependent internal quantum efficiency (IQE(T)) measurements were performed. The spectral response of the sample is measured within a temperature range from 100 K to 300 K. A reference cell and reflectance measurements of the sample at room temperature are used to calculate the internal quantum efficiency. From these measurements the temperature-dependent carrier

diffusion length and thus the minority carrier lifetime can be extracted.

HL 92.13 Thu 16:00 Poster A

Evolution of the performance parameters of Cu(In,Ga)Se2 solar cells during light soaking at different temperatures — •Johannes Schoneberg, Jörg Ohland, Janet Neerken, Jan Keller, Jürgen Parisi, Maria Hammer, and Ingo Riedel — Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Among all thin film photovoltaic technologies high-efficiency solar cells based on Cu(In,Ga)Se2 (CIGSe) absorber layers demonstrate the highest power conversion efficiencies around 20% . Metastabilities in device performance of CIGSe solar cells might lead to considerable light- or heat-induced variation of the solar cell parameters and therefore the efficiency. The fact that devices from different manufacturers exhibit more or less pronounced metastable behavior with different dynamics makes the topic interesting for a detailed analysis. A systematic study in which CIGSe solar the transient performance is monitored during light soaking, annealing and operation at different voltage bias will promote a more general understanding of the metastable device behavior. In this work CIGSe solar cells were light soaked at different light intensities and activation temperatures, while the performance parameters are monitored in a time series. From the results we intend to derive the activation energy between the relaxed and the light soaked states.

HL 92.14 Thu 16:00 Poster A

Investigation of defect energies of co-evaporated CIGSe solar cells — •Nils Neugebohrn, Maria S. Hammer, Christiane Stroth, Janet Neerken, Jan Keller, Jürgen Parisi, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

$CuInGaSe_2$ thin film solar cells are a promising candidate for the next generation low-cost and high efficiency solar cells. However, the relation between defect energies and the metastable/transient behavior of the performance is still an unsatisfyingly resolved issue. In CIGSe solar cells various anomalies are observed, which can provide insights in present defect dynamics, recombination mechanisms or possible transport barriers. Examples are the so called roll over and cross over effects in temperature dependent current-voltage characteristics (IV(T)) and shifting defect energies in deep level transient (DLTS) and admittance spectroscopy (AS(T)) depending on the conditioning of the solar cell prior to the measurement. In order to accurately investigate the impact of (pre-) conditioning, the defined initial or relaxed state of high efficiency CIGSe solar cells have been characterized by aforementioned methods. The results of this study and first results for cells in metastable conditions are presented.

HL 92.15 Thu 16:00 Poster A

Thin film GaN/Cu2O heterojunction solar cells — •Philipp Hering, Julian Benz, Daniel Reppin, Martin Becker, and Bruno Meyer — 1. phys. Inst., JLU-Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

Due to its high absorption coefficient, non-toxicity, and the abundance of its composing elements, cuprous oxide (Cu2O) is a promising absorber material in photovoltaic devices, even despite of the relatively large band gap (2.17 eV). With increasing success, more attention has recently been paid to Zinc Oxide/Cuprous Oxide heterojunctions. At higher forward voltages, however, the large conduction band offset impedes the minority carrier current across the interface: The theoretically attainable efficiency is decreased by about 50%. As a way out, we chose Gallium Nitride as window layer: It offers a conduction band offset of less than 0.2 eV in relation to Cu2O. Our cells were manufactured at room temperature by radio frequency sputter deposition of cuprous oxide, utilizing a copper target under addition of oxygen on top of Gallium Nitride templates. The templates consisted of a thin layer of GaN:Si, grown on a sapphire substrate by metal organic chemical vapor deposition. The sputtering was followed up by photolithographic structuring. For device characterization Current/voltage curves were obtained under AM1.5g illumination, different light intensities, as well as various temperatures, and the external quantum efficiency measured.

HL 92.16 Thu 16:00 Poster A

Optical and electrical characterization of InP-based InGaAsP/InGaAs low bandgap multijunction solar cells — •Anja Dobrich[1], Klaus Schwarzburg[1], Agnieszka Paszuk[2], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [2]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Ilmenau — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

Since III-V semiconductor concentrator solar cells grown by MOVPE become actually more attractive for terrestrial applications, it is a great issue to increase the efficiency while costs are reduced. III-V triple junction solar cells have demonstrated the highest conversion efficiencies (>41%) of any photovoltaic technology to date. Higher efficiencies can be achieved with a four-junction configuration, which has optimized band gaps. This can be realized with a mechanically stacked GaAs-based GaInP/GaAs top-tandem and an InP based InGaAsP/InGaAs bottom-tandem cell. Based on the latter two absorber materials, a low bandgap tandem solar cell with optimized bandgaps was developed. In the need for a suitable method to analyze our tandem cells, we developed an apparatus that allows for a fast and convenient evaluation of many cell performance parameters for illumination intensities equivalent up to 50 suns. The experimental setup makes it possible to measure all relevant data with the sample mounted on a probe station and to address each subcell of the tandem individually. Since the lifetime of minority carriers is one of the most important properties we analyzed the lifetime with time- and spatially-resolved photoluminescence.

HL 92.17 Thu 16:00 Poster A

Analysis of electronic subgap states in amorphous semiconductor oxides on the example of Zn-Sn-O — Wolfgang Körner[1], •Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg — [2]IAM-ZBS, Karlsruhe Institute of Technology

A molecular dynamics and density-functional-theory study of amorphous Zn-Sn-O with focus on the use as transparent conducting oxide material is presented. The amorphous structures generated by MD are subsequently relaxed using the local-density-approximation of DFT. The Zn/Sn ratio, the oxygen content and individual point defects are investigated concerning their thermodynamic and electronic properties and compared to the data for crystalline structures. Defect levels in the electronic band structure of ZnO are analyzed in terms of the density of states, which is calculated within the LDA and with a self-interaction-correction. We relate the electronic sub-gap states, which were recently observed experimentally, to structural features of the amorphous samples. We find the valence band tail, caused by the disordered O 2p orbitals, to be superimposed by deep defect states that can be assigned to under-coordinated O atoms. Doping with H atoms is found to suppress these states and improves the transparency. The deep levels below the conduction band arise mainly from under-coordinated Sn atoms or Zn–Sn pairs. The addition of oxygen can be a possible route to reduce such defect levels.[2]

[1] W. Körner, P. Gumbsch and C. Elsässer, PRB (2012) accepted.
[2] W. Körner and C. Elsässer, Thin Solid Films (2012) submitted.

HL 92.18 Thu 16:00 Poster A

Defect states in amorphous silicon nitrides: a-$Si_3N_xH_y$ — •Leif Eric Hintzsche[1], Gerald Jordan[1], Martijn Marsman[1], Machteld Lamers[2], Arthur Weeber[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]ECN Solar Energy, P.O. Box 1, 1755 ZG Petten, Netherlands

Amorphous silicon nitrides are commonly deposited as passivation layers on Si based solar cells with their stoichiometries depending mainly on the applied deposition process. By using ab initio molecular dynamics simulations, we investigated important structural and electronic properties, such as atomic coordination and electronic defect states, for different silicon nitride stoichiometries. We found two dominant defect classes in silicon nitrides: (a) under-coordinated Si atoms and (b) states localized on Si-Si bonds. Furthermore, we observed that in sub-stoichiometric silicon nitrides, percolation networks with longer Si chains lead to a considerable number of delocalized defect states in the band gap. While hydrogen can passivate under-coordinated Si atoms, electronic defects related to the latter class are hardly changed. These findings suggest that the dominant defect class also changes depending on the stoichiometry and the concentration of hydrogen.

HL 92.19 Thu 16:00 Poster A

Formation energy of point defects with transition metal (TM = Cr, Mn and Fe) doped barium titanate from first-principles studies — Sanjeev K. Nayak[1], •Waheed A. Adeagbo[1], Hans T.

Langhammer[2], and Wolfram Hergert[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle, Germany — [2]Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, Kurt-Mothes-Str. 2, 06120 Halle, Germany

We study the electronic properties of substitutional doped transition metal (TM = Cr, Mn and Fe) in barium titanate from the first-principles studies. We explore the stability of different valency states for the TM dopants which are probabilistic in experimental conditions. For such a consideration, we have modeled the system by charged supercells and also by possible charge compensation mechanism through the presence of oxygen vacancy (V_O). The analysis on the stability of defects is done by comparing the formation energy of defects. The regular expression of the Zhang-Northrup formulation for the formation energy of charge defects is used in our calculation together with the band gap correction. We use the Vienna *ab initio* simulation package (VASP). The supercell consists of 3×3×1 periodic repetition of hexagonal $BaTiO_3$ unit cell, which is the crystal structure of about 2 mol% TM-doped material at room temperature and normal pressure, and constitute of 54 functional units of $BaTiO_3$ where one Ti ion is substituted by a TM ion. Thus the defect concentration we are dealing with is about 1.85 mol% and this is in the range of experimental limits.

HL 92.20 Thu 16:00 Poster A

Metal organic chemical vapor deposition of GexSbyTez layers grown by using degermane — •Sally Riess[1,2], Daniela Schlösser[1,2], Michael Lübben[1,2], Toma Stoica[1,2], Martina von der Ahe[1,2], Kamil Sladek[1,2], Anna Haab[1,2], and Hilde Hardtdegen[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

GexSbyTez (GST) films grown on Si(111) substrates by epitaxy tend to be polycrystalline and therefore rough. Especially the incorporation of Germanium in the films is problematic. Thin and smooth film surfaces are however a prerequisite for memory applications. In the past we demonstrated that the metal organic chemical vapor deposition (MOCVD) growth of highly mismatched III/V materials such as InAs/GaAs can be accomplished conformally, if a low temperature growth process is used. This knowledge is transferred to MOCVD growth of GST. To this end as a Ge precursor digermane was employed which is expected to decompose at low temperatures. Commercial sources for Sb (triethylanthimony) and Te (diethyltellur) were chosen, which are suitable for low temperature deposition. At first the growth of Sb2Te3 layers was optimized. Than digermane was added to the growth process. Growth was evaluated by SEM, XRD and Raman measurements. It was found that GST can be deposited at the same conditions as Sb2Te3. SEM pictures show well coalesced, trigonal crystalline structures and XRD measurements verify the integration of Ge. The influence of growth parameters on layer growth will be presented.