

HL 71: Energy materials: Silicon-based photovoltaics

Time: Wednesday 15:00–17:15

Location: POT 151

HL 71.1 Wed 15:00 POT 151

Strained Lonsdaleite Silicon as a Potential Absorber for Photovoltaics — ●CLAUDIA RÖDL^{1,2,3}, TOBIAS SANDER^{2,3}, and FRIEDHELM BECHSTEDT^{2,3} — ¹Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France — ²Institut für Festkörperteorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — ³European Theoretical Spectroscopy Facility (ETSF)

Si in the diamond structure is one of the the key materials in photovoltaics, since it is abundant in nature and can be grown in extremely good quality. However, its fundamental band gap of 1.2 eV is indirect and only phonon-assisted absorption occurs in the visible spectral range. The direct absorption edge at 3.2 eV lies in the ultraviolet spectral region. Today a large variety of Si polymorphs is known, whereof some are semiconductors with direct gaps smaller than 3.2 eV.

Here, we calculate the optical absorption spectrum of Si in the lonsdaleite structure, also known as wurtzite Si, one of the most promising candidates for strong absorption in the visible spectral range. It features a direct band gap of 1.6 eV matching ideally with the solar spectrum. The quasiparticle band gap and the dielectric function including excitonic effects are calculated from first principles by many-body theory (*GW* method, Bethe-Salpeter equation). The optical absorption at the onset is compared to the absorption of diamond Si and discussed in terms of dipole-allowed and forbidden transitions. We study in detail the influence of hydrostatic pressure, uniaxial, and biaxial strain on the band gap and the optical absorption.

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Passivation of Silicon surfaces by Aluminum oxide layers: a DFT simulation study — ●FRANCESCO COLONNA^{1,2} and CHRISTIAN ELSÄSSER^{1,2} — ¹Albert-Ludwigs University, Freiburg Materials Research Center (FMR), Freiburg, Germany — ²Fraunhofer IWM, Freiburg, Germany

By the Atomic Layer Deposition of Aluminum oxide on a Silicon (100) surface, followed by a heat-treatment, it is possible to obtain an excellent surface passivation [1], which is expected to play a significant role in future photovoltaic application.

In the present study we investigate the interplay between the electronic structure at the interface and the local atomic environments of Aluminum oxide by means of density functional theory (DFT) simulation methods. Observations show that passivation is associated with a change in the proportion of local tetrahedral and octahedral cation coordination in the passivation layer. We model a number of stoichiometric or oxygen-rich interfaces between Silicon and *k*-Alumina, which entails both tetrahedra and octahedra. We also study the role played by additional Hydrogen at the interface. We relate the local features of the interface to the presence of electronic defect levels in the band gap, as computed by means of a self-interaction corrected [2] local-density approximation of DFT.

[1] G. Agostinelli et al., *Solar Energy Materials and Solar Cells* 90 (18-19), 3438-3443 (2006). [2] W. Körner and C. Elsässer, *Physical Review B* 81, 085324 (2010).

HL 71.3 Wed 15:30 POT 151

Electronic properties of nano-textured ‘black’ silicon — ●MANUEL SALZBERGER, MICHAEL ALGASINGER, SVETOSLAV KOYNOV, and MARTIN STUTZMANN — Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Nano-textured silicon, also referred to as black silicon (b-Si), shows a reflectivity below 5% in the whole range of Si absorption [1]. Furthermore, the nano-texture exhibits efficient light trapping effects, making it interesting for application in thin film solar cells. However, all black Si solar cells reported up to now show a poor external quantum efficiency in the short wavelength range due to elevated surface recombination. Besides the enlarged surface area, also the potential distribution within the nano-texture can affect the recombination rate.

Electrical measurements of nano-textured thin Si films were performed in order to investigate the influence of the structure depth on the electronic properties. The b-Si nano-textures were prepared with an Au-catalyzed wet-chemical etch process. Cross-sectional scanning electron microscopy images show a nano-texture consisting of c-Si hillocks, reaching deep into the substrate. From the comparison with a

planar reference sample, the influence of the nano-texture on the electrical conductivity will be investigated. From these findings, a better knowledge of the potential distribution within the nano-texture and, thus, a possible reduction of the surface recombination can be realized.

[1] S. Koynov, M. S. Brandt, and M. Stutzmann, *Appl. Phys. Lett.* 88, 203107 (2006).

HL 71.4 Wed 15:45 POT 151

Subnanometer thin silicon oxide films for the application as passivating interlayer in silicon heterojunction solar cells — ●WENJIA LU, CASPAR LEENDERTZ, HEIKE ANGERMANN, LARS KORTE, and BERND RECH — Helmholtz-Zentrum Berlin, Institute for Silicon Photovoltaics, Kekuléstr. 5, 12489 Berlin, Germany

Subnanometer thin silicon oxide (SiO_x) has previously been applied as interlayer between crystalline silicon (c-Si) wafers and hydrogenated amorphous silicon ((p)a-Si:H). To optimize such thin SiO_x passivation layers, oxidations on silicon wafers with different crystal orientations were performed by different oxidation methods. Native oxide and wet-chemical oxides of different thickness and after different chemical wafer pre-treatment processes are compared. The layer thickness (d_{ox}) was measured with spectral ellipsometry, while field-dependent photovoltage measurements and minority charge carrier lifetimes have been applied in order to assess the interface passivation quality and to determine the interface defect density (D_{it}) and charge (Q_{it}). For the native oxides a correlation between the defect density and the charge indicates that the overall charge is dominated by electrons trapped in defects. This relationship cannot be found for the wet-chemical oxides which show superior passivation quality. The highest passivation quality is obtained for the (111) surfaces after NH₄F pre-treatment for SiO_x layers of only 0.5 nm thickness. With a low D_{it} , a negative Q_{it} that supports emitter band bending and a low thickness, this wet-chemical oxide seems most suitable to be used as a buffer layer between the n-type c-Si absorber and the (p)a-Si:H emitter.

HL 71.5 Wed 16:00 POT 151

Comparison of Room Temperature Electroluminescence and Photoluminescence from Silicon Solar Cells — ●BEATRICE PÖTSCHICK, KARSTEN KURASCH, and JÖRG WEBER — Institut für Halbleiterphysik, Dresden, Germany

A set up for the detection of spatially- and spectrally-resolved luminescence from Si solar-cells was constructed. A thermoelectrically-cooled InGaAs-camera was connected to a spectrometer for investigations in the spectral range from 900 to 1700nm. After validating the performance of our system, we discuss the results of electroluminescence experiments on Si solar cells. The results are compared to spectrally resolved photoluminescence measurements from the same solar cells. Clear spectral differences of the two techniques are detected and related to different areas on the solar cell. The origin of these differences will be discussed.

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Iron-related traps in near-junction volume of crystalline silicon solar cells — ●TEIMURAZ MCHEDLIDZE and JÖRG WEBER — Technische Universität Dresden, 01062 Dresden, Germany

Deep traps of majority carriers were detected recently in the near-to-junction volume (NJV) of fully processed crystalline solar cells [1]. The traps were detected using mesa-structured n+p-junctions prepared on the processed Si solar cells by deep level transient spectroscopy (DLTS). In this report we present an investigation of the trap formation at various stages of the standard solar cell fabrication process. The samples fabricated from the Czochralski-grown crystals with various initial iron contents were investigated. Total iron content in the samples was determined by DLTS in the as-grown samples subjected to high-temperature annealing followed by fast quenching. The NJV trap density at various steps of the solar cell fabrication process correlated with the iron content in the starting material and dropped strongly with the distance from the junctions. The traps were detected already after phosphorus diffusion and further fabrication processes varied their density depending on the initial iron content in the wafers. The results suggest that the iron-related NJV traps are formed during/after the phosphorus diffusion process. Our results could help in tailoring the solar cell fabrication process parameters to the content

of contaminants in the feedstock.

[1] T. Mchedlidze, L. Scheffler, J. Weber, M. Herms, J. Neusel, V. Osinniy, C. Möller, and K. Lauer, *Appl. Phys. Lett.*, 103, 013901 (2013).

HL 71.7 Wed 16:30 POT 151

Formation of near junction and bulk traps in crystalline silicon solar cells — •TEIMURAZ MCHEDLIDZE¹, CHRISTIAN MÖLLER², KEVIN LAUER², and JÖRG WEBER¹ — ¹Technische Universität Dresden, 01062 Dresden, Germany — ²CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Utilization of low quality feedstock for Si crystal growth was acknowledged as a valuable strategy for further price reduction of solar cell production. However, this strategy requires correct determination of the acceptable limits for the feedstock cleanness and relevant tailoring of the solar cell fabrication process. Recently we reported on influence of the fabrication steps on the bulk lifetime in the wafers produced from the various feedstock materials [1]. Deep traps of majority carriers were detected in the similar samples in near to the junction volume (NJV) using mesa-structured n+p-junctions prepared from the processed Si solar cells by deep level transient spectroscopy (DLTS) [2]. In this report we compare results from lifetime measurement and from DLTS for various quality crystals at various stages of solar cell fabrication process. Apparently, the NJV traps differ from those formed in the wafer bulk. However, in the both cases the trap densities correlate with the total content of iron in the crystals. The analyses of our results allow suggesting changes to the solar cell fabrication processes minimizing the influence of iron contamination.

[1] K. Layer, et al., *Energy Proc.*, 38, 589 (2013) [2] T. Mchedlidze, et al., *Appl. Phys. Lett.*, 103, 013901 (2013)

HL 71.8 Wed 16:45 POT 151

Nanostructuring of silicon and surface passivation of silicon nanostructures for organic-inorganic hybrid solar cell absorbers — •STEFANIE GREIL¹, XIN ZHANG¹, MATTHIAS ZELMEIER¹, SILVIA JANIEZ², NORBERT NICKEL¹, and JÖRG RAPPICH¹ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin (Germany) — ²Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 69, 14476 Potsdam (Germany)

Metal assisted chemical etching (MACE) using Ag nanoparticles as cat-

alysts is an outstanding method for nanostructuring Si wafers to modify its optical properties for photovoltaic applications. To obtain regular nanostructure arrays, MACE processes are combined with shadow nanosphere lithography. Self assembled polystyrene nanosphere masks were realized by Langmuir-Blodgett techniques. For further variations in diameter and spacing of the Si nanostructures, reactive ion etching of the polystyrene nanosphere masks is applied. As MACE processes always lead to etching induced surface defects in the resulting Si nanostructures, suitable post-etching surface treatments are necessary. As a direct surface passivation process, the application of electrochemical functionalization by methyl groups is examined. Another approach is to remove the damaged surface of the Si nanostructures by subsequent electrochemical oxidation and Si oxide dissolution. Finally, the influences of the nanostructured substrate and its different surface passivation are studied on hybrid solar cells with a thiophene/Si interface.

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Surface characterization of arsenic terminated Si(111) substrates with MOVPE for III-V nanowire solar cells — •WEIHONG ZHAO¹, AGNIESZKA PASZUK¹, MATTHIAS STEIDL¹, SEBASTIAN BRÜCKNER¹, ANJA DOBRICH², JOHANNES LUCZAK², PETER KLEINSCHMIDT^{1,3}, HENNING DÖSCHER¹ und THOMAS HANNAPPEL^{1,2,3} — ¹Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — ²Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — ³CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

III-V nanowires grown on Si(111) substrates by metal-organic vapor phase epitaxy (MOVPE) enable a promising new solar cell concept meeting the demands of high-quality-low-cost photovoltaics. GaP buffer layers grown on Si(111) substrates represent suitable quasi-substrates since GaP is almost lattice-matched to Si. Apparently, preparation of atomically flat Si (111) surfaces is an essential step as a precondition for adjacent GaP heteroepitaxy. However, little is known about preparation and surface properties of Si(111) surfaces in MOVPE with H₂ ambient. A contamination-free transfer system enabled us to study the MOVPE prepared surfaces with numerous UHV based surface science tools. We found that a dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces. Moreover, the GaP heteroepitaxy leads to an unfavorable A-type surface for growing vertical nanowires. We successfully applied a controlled arsenic termination procedure during the epitaxy for changing the surface polarity.