DS 22 Optische Spektroskopie dünner Schichten II

Zeit: Dienstag 14:30–16:45 Raum: TU H110

DS 22.1 Di 14:30 TU H110

Optical response of a π-conjugated molecular monolayer adsorbed on Si(001): A *first-principles* study — •Andreas Hermann, Wolf G. Schmidt, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich–Schiller–Universität, Max–Wien–Platz 1, 07743 Jena, Germany

Organic functionalization of semiconductor surfaces has become important for developing new semiconductor-based devices. The modification of the surface optical response for the prototypical system of the π-conjugated molecule 9,10–phenanthrenequinone adsorbed on Si(001) is investigated by means of *first-principles* calculations . Optical properties are calculated within the independent-particle approximation from all-electron wave functions obtained by the projector augmented wave method (PAW). Structural data and Reflectance Anisotropy Spectra (RAS) agree well with recent experimental findings [1,2]. The detailed analysis of the optical signal shows that intramolecular π–π^* transitions as well as adsorption–modified Si bulk states contribute to the surface spectrum. The calculations illustrate the sensitivity of optical spectroscopy to molecular adsorption but demonstrate clearly that a naive interpretation of the spectrum in terms of gas-phase molecular data fails.

[1] L. Fang *et al.*, Surf. Sci. **514**, 362 (2002).
[2] C. Hacker and R. J. Hamers, J. Phys. Chem. B **107**, 7689 (2003).

DS 22.2 Di 14:45 TU H110

Dielektrische Simulation der optischen Eigenschaften von TCO-Schichten — •Dieter Mergel und Zhaohui Qiao — Universität Duisburg-Essen, Fb Physik, AG Dünnschicht-Technologie, 45117 Essen

Transmissions- und Reflexionsspektren dünner Schichten aus In(2)O(3):Sn [1] und ZnO:Al [2] lassen sich sehr gut mit einer dielektrischen Funktion simulieren, die einen harmonischen Oszillator für die Interbandübergänge, ein Drude-Modell mit Energie-abhängigem Streuterm und ein angepasstes Modell für die Bandkantenabsorption enthält.

Aus dem Drude-Term können Werte für Ladungsträgerdichte und - Beweglichkeit ermittelt werden, die mit Hall-Effekt-Werten verglichen werden und Aussagen über effektive Massen oder Korngrenzen-Widerstände erlauben.

Ellipsometrische Spektren können mit derselben dielektrischen Funktion simuliert werden, wenn man eine wenige nm dicke Oberflächenschicht ins Modell einführt, die zur Hälfte aus dem Volumenmaterial und Luft besteht (entsprechend einer Oberflächenrauhigkeit).

[1] D. Mergel, Z. Qiao, J Phys D: Appl. Phys. 35 (2002) 794-801 [2] Z. Qiao, D. Mergel, C. Agashe, submitted for publication.

DS 22.3 Di 15:00 TU H110

Reflectance anisotropy spectroscopy as a versatile tool for the development and control of MOVPE growth processes for devices — •Martin Zorn[1], Thomas Zettler[2], and Markus Weyers[1] — [1]Ferdinand-Braun-Institut für Höchtsfrequenztechnik (FBH), Gustav-Kirchhoff-Str. 4, D-12489 Berlin — [2]LayTec GmbH, Helmholtzstr. 13/14, D-10587 Berlin

Reflectance anisotropy spectroscopy (RAS) in combination with reflectance (R) measurements has made the way out of research into production of layer structures for compound semiconductor devices by metal-organic vapour phase (MOVPE). The sensitivity of RAS to surface processes (e.g. oxide desorption and interface formation) as well as bulk properties (e.g. composition and doping concentration) and the possibility to perform measurements *in-situ* during the semiconductor growth process is the essential advantage in comparison to ex-situ techniques like x-ray diffraction and C/V profiling.

This contribution focuses on the usage of the RAS and R technique for the growth of layer structures for laser diodes. In these structures a high reproducibility of layer parameters like composition, doping profile and emission wavelength is needed to achieve the stringent requirements of the final laser device which increase steadily. Examples will be given for *in-situ* measurements of e.g. composition, doping profiles and emission wavelength during MOVPE growth in a production-like environment. For the layer structures presented in this work the focus is mainly on the material systems AlGaAs, AlGaInP and GaAsP. Furthermore, the reproducibility of the growth process and the measurement itself is discussed.

DS 22.4 Di 15:15 TU H110

New opportunities for RAS analysis of metal surfaces and thin films — •Peter Zeppenfeld, Lidong Sun, and Michael Hohage — Institut für Experimentalphysik, Universität Linz, Austria

During the last decade, reflectance anisotropy spectroscopy (RAS) has proven to be a powerful tool for the analysis of metal surfaces, in addition to its well established application to semiconductor surfaces and thin films. Various issues such as the adsorption and growth, surface restructuring and the morphological changes during ion sputtering or thermal treatment can be conveniently monitored in situ and in real time using the RAS technique. Yet, the electronic structure and the associated optical properties of metal surfaces are quite different from those of semiconductors. This introduces new challenges for the understanding of the origin and the quantification of the RAS signals from metal surfaces, but it also offers new opportunities and applications. For instance, the presence of delocalized (free electron like) surface states on metal surfaces makes RAS an extremely sensitive tool for studying adsorption kinetics and ordering phenomena. On the other hand, bulk derived contributions to the optical anisotropy are sensitive to thin film and surface stress and can thus be used to characterize the growth mode and morphological changes of thin metal films through the associated characteristic strain/stress variations. Finally, we demonstrate that apart from morphological changes, RAS also allows to follow the evolution of the electronic band structure of a growing thin metal film in a layer by layer fashion.

DS 22.5 Di 15:30 TU H110

In-situ RAS study of para-sexiphenyl film growth on metal and oxide surfaces — •L.D. Sun[1], M. Hohage[1], Y. Hu[1], K. Maschek[1], P. Zeppenfeld[1], S. Berkebile[2], F.P. Netzer[2], and M.G. Ramsey[2] — [1]Institut für Experimentalphysik, Johannes-Kepler-Universität Linz, Austria — [2]Institut für Experimentalphysik, Karl-Franzens-Universität Graz, Austria

Para-sexiphenyl (P6P) is an aromatic molecule, which is classified as a wide gap organic semiconductor with an electronic band gap of 3.1 eV. The molecule which consists of a linear chain of six linked benzene rings gives a strong intrinsic electronic and optical anisotropy. This fact allows probing the orientation of the P6P molecules by monitoring the polarization dependence of the optical absorption. Reflectance Anisotropy Spectroscopy (RAS), on the other hand, is a powerful tool to study the lateral optical anisotropy and its evolution of the growing thin films and the substrate beneath. Here, we present our RAS in-situ investigation of P6P films growth on oxide (TiO_2(110)) and metal (Cu(110)) surfaces. The films have been prepared by physical vapour phase deposition in UHV under diverse conditions. Pronounced optical anisotropies arising from the optical absorption of P6P have been observed for the distinct films. In fact, based on the behaviour of the RAS feature contributed by the HOMO to LUMO transition of the P6P molecules, important information about the orientation and the conformation of the P6P molecules in the films can be obtained directly. Furthermore, the RDS is very sensitive to small quantities of P6P and therefore well suited for the investigation of the initial stages of P6P growth.

DS 22.6 Di 15:45 TU H110

Potential fluctuations in compensated Cu(In,Ga)Se_2 - A photoluminescence study — •Niklas Rega, Susanne Siebentritt, Juergen Albert, and Martha Lux-Steiner — Hahn-Meitner-Institut Berlin, Glienicker Str. 100, D-10405 Berlin

Cu(In,Ga)Se_2 is a compound semiconductor which belongs to the family of chalcopyrites. They are interesting materials for application(solar cells achieve efficiencies of 19.5%) and a fascinating topic for fundamental investigations due to their unique phase and defect behaviour. Intrinsic defects are doping the chalcopyrite. Therefore metal organic vapour phase epitaxy is used for the growth to ensure good composition control.
High efficiency Cu(In,Ga)Se_2 solar cells are fabricated under Cu-poor conditions, i.e. $[Cu]/([Ga]+[In]) < 1$. The photoluminescence (PL) spectra of $CuGaSe_2$ and $CuInSe_2$ films grown under Cu-poor conditions are characterized by a broad asymmetric luminescence. Temperature and power dependent PL measurements show that the broadening of luminescence is due to a donor-acceptor-pair (DAP) transition in the presence of locally fluctuating potentials due to compensation. Here we present a PL study on Cu-poor grown epitaxial Cu(In,Ga)Se_2-layers with varying

[Ga]-content. The aim of this contribution is the quantification of the potential fluctuations in dependence of the [Ga]-content. The depth of the fluctuating potentials is estimated. For $CuGaSe_2$ we get a mean depth of 70meV and for $CuInSe_2$ of 20meV. The influence of fluctuations in the [Ga]-content, which causes a fluctuation of the band gap energy, has to be taken into account for Cu(In,Ga)Se_2.

DS 22.7 Di 16:00 TU H110

Photoluminescence Excitation Spectroscopy of highly compensated $CuGaSe_2$ — •Susanne Siebentritt, Alexander Zajogin, Niklas Rega, and Martha Lux-Steiner — Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin

The interest in $CuGaSe_2$ is twofold: it is an attractive absorber material for thin film tandem solar cells and it shows a unique behaviour concerning its native defects, which have very low formation enthalpies, concerning its phase behaviour and its grain boundaries. The material used in solar cells is grown under Cu-poor conditions. Previous work has shown that this material is highly compensated and shows spatial potential fluctuations. To investigate these fluctuations the absorption of the band tails needs to be measured. Since grain boundary free material today can only be obtained by epitaxy on GaAs no transmission spectroscopy is possible. Therefore the band tail absorption and its overlap with luminescence is investigated by PLE (photo luminescence spectroscopy). From the overlap the amplitude of the fluctuations is determined to at least 70 meV. The absorption spectra obtained by PLE depend strongly on the detection wave length. This is due to the fact that different detection wave lengths probe different depths of the fluctuations. Interestingly the same effect has been observed in $CuGaSe_2$ grown under Cu excess where no potential fluctuations are expected. A critical review of PLE as a measure for the absorption will be given together with a comprehensive analysis of the potential fluctuations in $CuGaSe_2$.

DS 22.8 Di 16:15 TU H110

VUV spectroscopic ellipsometry of cytosine and functionalized cytosine using synchrotron radiation — •Y. Suzuki[1], O. D. Gordan[1], S. D. Silaghi[1], A. Schubert[1], W. R. Thiel[1], C. Cobet[2], W. Braun[3], and D. R. T. Zahn[1] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institute of Spectrochemistry and Applied Spectroscopy, D-12489 Berlin, Germany — [3]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, D-12489 Berlin, Germany

DNA base molecules have potential as materials in organic electronics. However, there is so far only very little work on the properties of the DNA bases in the form of layers on inorganic substrates. Here we report on the optical properties, i.e. dielectric function, of cytosine and a functionalized variant, 1-allylcytosine, obtained by spectroscopic ellipsometry in the VUV photon energy range (4 - 9.5 eV). The samples were prepared by organic molecular beam deposition onto hydrogen passivated silicon substrates under ultra-high vacuum conditions. Typical thicknesses of the layers studied were in the range of 700-900 nm. The results reveal that the optical response changes significantly as a result of the addition of the functional group to the molecule, while density functional theory based ab-initio calculations predicted very similar absorption spectra.

DS 22.9 Di 16:30 TU H110

Characterization of GaN/$Al_xGa_{1-x}N$ quantum well structures by spectroscopic ellipsometry and photoluminescence — •U. Rossow, D. Fuhrmann, T. Retzlaff, N. Riedel, and A. Hangleiter — TU Braunschweig, Inst. f. Techn. Physik, 38106 Braunschweig; b.postels@tu-bs.de

In this contribution we combine the optical methods spectroscopic ellipsometry and photoluminescence (PL) to characterize $Al_xGa_{1-x}N$-layers, GaN/$Al_xGa_{1-x}N$ single and multi quantum-well (SQW, MQW) and GaN-AlN MQW structures. The QW structures are promising for various devices such as LEDs or lasers in the UV range. Challenges are on one hand the crystalline quality of $Al_xGa_{1-x}N$ as well as the high strain due to lattice and thermal mismatch in the heterostructures. On the other hand it turned out that thickness (quantum wells) and composition x_{Al} need to be carefully controlled in order to achieve reproducible emission wavelengths. To determine both parameters ellipsometry is usually thought to be the best choice. However, for the GaN SQW structures which are typically 1-3nm grown with $Al_xGa_{1-x}N$ barriers of typically $x_{Al} \sim 0.23$ we observe no contribution directly related to QW transitions. This is in contrast to GaN MQW structures where features appear in the spectra. All investigated samples show strong PL signals indicating that material quality is not the cause. It is likely that for such thin SQW structures the signal is too weak to be detected at room temperature (typical signal-to-noise ratio). The problem is even worse due to the fact that strong piezoelectric fields exist in the quantum wells and therefore spectral features tend to be weaker.