DS 21 FV-internes Symposium Optische Spektroskopie von dünnen Schichten und Grenzflächen

Zeit: Dienstag 09:45–13:30 Raum: TU H110

Hauptvortrag DS 21.1 Di 09:45 TU H110

Real-time optical diagnostics for epitaxial growth — •D. E. Aspnes — Physics Dept., NC State University, Raleigh, NC 27695-8202

Optical diagnostics are currently the only means of assessing the epitaxial growth of materials in the relatively high pressure environments characteristic of organometallic chemical vapor deposition (OMCVD). These diagnostic techniques include reflectance-anisotropy (-difference) spectroscopy (RAS/RDS) for determining surface reconstructions and terminations, laser light scattering (LLS) for detecting the onset of microscopic roughness, and spectroscopic ellipsometry (SE) for measuring compositions and thicknesses of depositing layers. As a result of the needs of the semiconductor industry, the capabilities of SE in particular have been significantly enhanced in the last several years, with the result that the rotating-polarizer and -analyzer configurations that dominated SE for the last 30 years are being replaced by rotating-compensator designs. When coupled with photodiode-array detectors, rotating-compensator systems allow highly accurate SE data to be obtained at rates of the order of Hz, significantly extending capabilities for growth assessment as well. As a general example I discuss the use of SE and LLS in an integrated OMCVD reactor to optimize the heteroepitaxial growth of GaSb on GaAs, which allowed the production of material where interface defects were limited to those needed to accommodate the 7.8% lattice mismatch between substrate and overlayer. Analysis of data obtained at 1 s (0.2 nm growth) intervals during the critical initial stages of heteroepitaxy showed that in this case heteroepitaxy initiated as GaSb islands in GaAs.

Hauptvortrag DS 21.2 Di 10:30 TU H110

Ab-initio calculations of electronic and optical properties of surfaces — •Olivia Pulci — INFM, Department of Physics, University of Rome, Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy

The microscopic study of complex systems has nowadays reached a high level of accuracy that allows for a deep understanding of the electronic excitations. Ab-initio description of experiments such as direct or inverse photoemission, optical absorption, electron energy loss, have become possible thanks to the huge progress in theory and the increased computational power. Charged excitations, as well as neutral excitations, can now be studied within the Many-Body Perturbation Theory based on the Green's function formalism. Optical spectra can be calculated with inclusion of the electron hole interaction by solving the Bethe Salpeter equation (BSE) within the framework of Green's function theory. Moreover, optical spectra can be nowadays also well described within the Time Dependent Density Functional Theory (TDDFT).

In this seminar we will present results for the electronic structure and reflectance anisotropy of diamond and silicon surfaces within DFT, GW, and BSE approach. Results for the optical spectrum of Si(111)2x1, calculated within the TDDFT approach will be also discussed.

Hauptvortrag DS 21.3 Di 11:15 TU H110

Optical analysis of monolayers at surfaces and interfaces — •V. Wagner — School of Engineering and Science, International University Bremen, Campus Ring 8, D-28759 Bremen, Germany

Controlling of surface and interface properties is crucial for tailoring advanced materials, especially if the structure size in one or more dimensions approaches the nanoscale regime. Thus, analysis and modification of the last atomic layer is of crucial importance. Optical probes offer the advantage of high spectral resolution and the possibility to analyze under liquid, vapor and vacuum environments. With emphasis on Raman spectroscopy and modulation spectroscopy various examples of analysis of structural and binding properties of such monolayers are discussed. Especially materials used in electronic applications, i.e. organic and inorganic semiconductors, are addressed. It is demonstrated how the orientation of surface reconstructions of II-VI semiconductors are determined by Raman spectroscopy or the modification of bonding properties is sensed of organic molecules, e.g. 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on top of metallic silver surfaces. Furthermore, modulation spectroscopy is applied to follow the changes of the electronic properties and provides complementary information to the vibrational data obtained by Raman scattering.

Hauptvortrag DS 21.4 Di 12:00 TU H110

Biomolecular layers on silicon studied by optical spectroscopy — •Dietrich R.T. Zahn — Institut für Physik, TU Chemnitz, D-09107 Chemnitz

Amongst biomolecules the DNA base molecules adenine, cytosine, guanine, and thymine may also find interesting applications in organic electronics. They have optical gaps in the near ultra-violet and have already been considered as charge transport molecules in organic field effect transistors. Still there is very little knowledge on their electronic and optical properties when deposited as layers on inorganic substrates. Here the optical properties of the DNA bases deposited on flat and vicinal, hydrogen passivated Si(111) substrates are studied using spectroscopic ellipsometry (SE) up to 9.5 eV photon energy employing synchrotron radiation and reflectance anisotropy spectroscopy (RAS). The results for the dielectric function reveal strong optical anisotropy for adenine and guanine while the other two molecules form layers with isotropic properties. The experimentally derived dielectric functions are compared to density functional theory calculations of the optical response. Particularly interesting is the RAS response of the DNA bases as a function of thickness when deposited on vicinal Si surfaces. Ordering in the layers is induced by the step and terrace structure of the vicinal Si substrates. Even though the molecular structure is not dramatically different the RAS response is very distinct and allows an unambigious identification of the bases.

Hauptvortrag DS 21.5 Di 12:45 TU H110

Infrared ellipsometry for structure analysis of organic films — •Karsten Hinrichs[1], Michael Gensch[1,2], Katy Roodenko[1], and Norbert Esser[1] — [1]ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [2]Gesellschaft zur Förderung angewandter Optik, Optoelektronik, Quantenelektronik und Spektroskopie e.V., Rudower Chaussee 29, 12489 Berlin, Germany

FT-IR reflectance methods such as infrared spectroscopic ellipsometry (IRSE) provide structural information of thin films by probing the reflectance for radiation differently polarized with respect to the plane of incidence [1-3]. From IRSE not only the real and imaginary part of the dielectric function is derived but also the depolarisation within the sample can be measured. Thereby the high analytical potential is based on (i) a non-contact and non-invasive measurement (ii) monolayer sensitivity (iii) identification of chemical bonds of the film and interface by vibrational absorption bands and (iv) optical modelling with respect to molecular orientations and structure. The high sensitivity and the high chemical information allowed valuable studies of ultra thin films and their interfaces (e.g. Nitrobenzene on Si(001), H/Si(001) and SiO_2/Si(001). [1] K. Hinrichs, D. Tsankov, E. H. Korte, A. Röseler, K. Sahre and K.-J. Eichhorn, Appl. Spectrosc. 56 (2002) 737 [2] N. A. Nikonenko, K. Hinrichs, E. H. Korte, J. Pionteck, K.-J. Eichhorn, Macromolecules 37 (2004) 8661 [3] K. Hinrichs, M. Gensch, A. Röseler, N. Esser, J. Phys.: Cond. Matt. 16 (2004) S4335