

### X-RAY STANDING WAVE MICROSCOPY PERMITS CHEMICAL MICROANALYSIS WITH ATOMIC RESOLUTION

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Compound materials with high perfection in crystallinity and a high degree of integration on a microscopic scale are becoming increasingly important in technology and technology driven research. Integration length-scales range from sub-micrometer for electronic to several micrometers for integrated optoelectronic devices, electro-mechanical systems, and sensors, etc. The optical and electronic properties of the underlying crystalline materials are tailored by the controlled combination or substitution of constituents with other elements to an increasing complexity. Characterizing such crystalline structures on the microscopic level with chemical sensitivity and atomic resolution is not an easy task. In the present work we introduce an advanced microprobe technique based on the XSW method demonstrating that structural analysis can be achieved with chemical sensitivity on a microscopic scale. We apply the XSW microscopy technique to study an epitaxially grown GaAs/Al<sub>0.1</sub>Ga<sub>0.9</sub>As/GaAs(001) heterostructure in cross-section determining the lattice location of individual elements on a microscopic scale. We focus the x-ray beam by a refractive lens into a micrometer slice and generate the XSW field by Bragg-reflection from the (220) diffraction planes of the cleaved sample. In this first demonstration, we analyze Al, Ga, and As, the constituent elements of the used structure confirming the substitutional location of Al with a resolution of about 10 pm, typical for conventional XSW measurements. The new micro-XSW technique will permit microscopic examinations of the crystalline structure of modern semiconductor devices with chemical sensitivity and structural resolution on the pm scale.

**Keywords:** X RAY STANDING WAVE, X RAY MICROSCOPY, HETEROSTRUCTURES

### SOFTWARE TO MANAGE THE SYNCHROTRON EXPERIENCE: EXPERIMENTAL CONTROL AND A DATABASE

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We have pioneered the integration of beamline and experimental control for synchrotron diffraction experiments. More recently we extended observation and control of experiments to experimenters who gain access through the World-Wide Web. We find that a surprising difficulty in high-throughput crystallography is organization of the data that result from synchrotron experiments.

These data include not only the measurements, but also the experimenter's personal data and a statistical record of the course of data processing, and possibly of structure solving. We are implementing a database system that is tightly integrated to the synchrotron experience, all the way from the beamtime request or structural genomics experiment, through to the data-collection and structure-solving process.

Typically, crystals that are brought to the synchrotron for analysis already have a heterogeneous assembly of data related to the preparation of the sample and preliminary x-ray studies. At the synchrotron the crystals are screened for x-ray diffraction, a collection strategy is developed, and the data are measured. After the synchrotron collection and primary reduction and scaling of the data, crystallographic analysis continues with phasing (MAD, SAD, MR) and model building. Throughout this process 'meta' data are produced: wavelength, heavy-atom absorption spectra, time-of-day, x-tal-to-detector distance, etc. Whether the user is involved in a high throughput structural genomics project, or is proceeding more conventionally, all of these data should remain accessible and documented. Our new system is designed to do this.

**Keywords:** SYNCHROTRON DATABASE SOFTWARE

### METHOD FOR POSITION SENSITIVE X-RAY ABSORPTION SPECTROSCOPY

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Position sensitive methods provide information about inhomogeneous samples. With position sensitive X-ray diffractometry for example polycrystalline samples could be characterized. Here a method for position sensitive X-ray absorption spectroscopy (XAFS) in transmission geometry will be presented. XAFS-measurements in fluoreszenz mode are already done. For XAFS measurements the sample is placed between two ionization chambers and the logarithm of the quotient of the intensities is plotted against the energy. For receiving position sensitive information (i.e. variation of spatial distribution of an element or differences in the oxidation state) a position sensitive detector is placed behind the second absorption chamber. In the experiments done until now an imaging plate was used, but it is also possible to use a CCD-camera. To increase the dynamic region of the detector the intensity of the second ionization chamber is used as monitor for the counting time. Measurements were done at the iron K-edge of thurmaline, an iron containing silicate.

**Keywords:** SYNCHROTRON RADIATION X-RAY ABSORPTION SPECTROSCOPY POSITION SENSITIVE

### POLARIZATION EFFECTS ON N-BEAM DIFFRACTION

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Simultaneously diffracted beams interference effects in crystals have been one of the key tools for a physical solution of the so-called 'phase problem' in the crystallographic structure determination. This and many other applications in materials science for simultaneous diffraction, also referred to as n-beam X-ray diffraction in crystals, have always been limited to the diffraction cases where the relative strength of the diffracted beams matches the requirements of each application. In this work, we demonstrated how the synchrotron radiation linear polarization state can be used as a critical variable in the simultaneous diffraction process that is able to completely change the relative strength of the beams. In particular, the intensity of one multiple beam peak was monitored as a function of the polarization and the peak, initially an umweganregung one, became a aufhellung peak.

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**Keywords:** SYNCHROTRON RADIATION, POLARISATION, X-RAY MULTIPLE DIFFRACTION