Atomic Configurations and Composition of the ZnSe(100)
Surface: Combined investigation by SXRD and XPS

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Triggered by recent progress in fabrication of optoelectronic devices and in injection of spin-polarized electrons into nonmagnetic semiconductors the interest in II-VI semiconductor thin films has strongly increased again. In this context the surface reconstructions of ZnSe, one of the model systems in the field of II-VI MBE, are of high relevance. Therefore this surface has been under intense examination for more than a decade. Methods used most frequently are low energy electron diffraction (LEED), x-ray photoemission spectroscopy (XPS) [1] and first principle-based calculations of the surface energy [2]. Two different reconstructions are known for the ZnSe (001) surface: A Se-rich (2x1) reconstruction is formed at ~320°C and changes to a c(2x2) reconstruction at higher temperatures. From experimental and theoretical results different models were established for both reconstructions, a Se-dimer model for the (2x1) and a Zn-vacancy model for the c(2x2) reconstruction. Very recent investigations with reflection high energy electron diffraction (RHEED-IV) [3] question the Zn-vacancy model and suggest a Se-vacancy structure which occurs during MBE growth on the c(2x2) reconstructed surface. For a clarification of this aspect and an exact structure determination we performed surface X-ray diffraction (SXRD) and XPS experiments at the beamlines BW2 and E1 at HASYLAB.

The samples were grown in a combined III-V/II-VI MBE-chamber at the University of Würzburg. The nominal thickness of the ZnSe layers was ≈150 nm. After cooling the samples under Zn-flux the c(2x2) reconstructed surfaces were capped with Se at room temperature and transported to HASYLAB under UHV conditions (p<10⁻⁹ mbar). The final preparation of both surface reconstructions was performed by desorption of the Se cap under different conditions:

- By to desorption at 320°C a weak (2x1) reconstruction is formed with broad superstructure spots indicating a very small domain size. It was not possible to measure SXRD data on this weak reconstruction. Since annealing at higher temperatures converts the surface to the c(2x2) reconstruction we tried to improve the (2x1) reconstruction (i.e. to increase the domain size) by careful annealing at 380°C under Se-flux (p = 3·10⁻⁸ mbar). This procedure yielded surface domains which were large enough to measure a SXRD data set of good quality. The data analysis for the (2x1) data set is in progress.

- Desorption of the Se cap at temperatures above 400°C (or annealing the sample at this temperature) results in a c(2x2) reconstructed surface showing very large domains (1000Å, evaluated from SPA-LEED spot profiles).

After preparation the sample was transferred into the UHV-chamber mounted at the surface diffractometer at the BW2 beamline. For the c(2x2) reconstruction extended in-plane and out-of-plane data sets were measured at a wavelength of $\lambda = 1.30$ Å with the angle of incidence of 0.3°. Fig. 1 and 2 show the in-plane and a part of the out-of-plane data set, respectively. These preliminary fit results demonstrate, that the essential features of the c(2x2) surface reconstruction can be described by the Zn-vacancy model shown in Fig. 3. However, minor discrepancies in the fit, indicated by obvious deviations of calculated and measured integer order rods and a relatively high value of 5.23 for $\chi^2$, still have to be eliminated to describe all details of the c(2x2) reconstruction. Further data analysis and testing of other models, in particular the Se-vacancy model, are still in progress.
To ensure the relevance of our results with respect to the c(2x2) reconstruction known from literature and to demonstrate that our sample preparation under Se flux is equivalent to the preparation in, e.g., the paper by Chen et al. [1], XPS measurements were performed after the SXRD measurements using the same samples. The transfer to the XPS-chamber at the E1 beamline was done under UHV. The measured Se 3d and Zn 3d core-level spectra show no significant differences to those of Ref. [1]. This work was supported by the Deutsche Forschungsgemeinschaft through SFB 410.

References