Surface x-ray diffraction of surface reconstructions on GaSb(001)

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GaSb(001) is an important semiconductor substrate, on which, mid- and long-wavelength lasers and photodetectors are grown. We report the successful investigation of two surface reconstructions on the GaSb(001) surface. An extensive amount of diffraction data has been collected in order to determine the in-plane and out-of-plane structure of these surface phases.

Introduction

GaSb is a technologically important zinc blende direct band gap semiconductor used for photonic applications in the long wavelength range. It is closely lattice-matched to InAs and AlSb, allowing the growth of band gap engineered device heterostructures. Besides its technological importance, it features peculiar growth kinetics [1] and a sequence of surface reconstructions that is different from the other III-V zinc blende structure semiconductors. These properties may open the way to use growth modes different from the established ones employed for the related materials. The ordered atomic array of the underlying crystal substrate imposes specific constraints on the atoms migrating, aggregating and crystallizing on the surface. Quantitative experimental data on the early stages of crystal growth are therefore of fundamental importance both to verify and further develop theoretical models as well as to find bottom-up approaches for the improved fabrication of microelectronic and nanoelectronic devices. X-ray diffraction is the tool of choice for in situ structural investigations of crystalline species, since x-rays only weakly interact with the sample. This same property also allows a reliable and quantitative interpretation of the results using the established and mature methods of x-ray analysis.

The specific designation of the surface reconstructions on GaSb(001) is still under debate, however, based on symmetry observed by reflection high-energy electron diffraction (RHEED), a (1 x 5) structure is observed at lower temperatures and a (1 x 3) structure is observed at higher temperatures. The (1 x 3) phase is perhaps most technologically relevant since it is on this surface that most devices are grown. Based on scanning tunneling microscopy (STM) measurements, investigators have reported two different (4 x 3) [2] structures that have been found to co-exist when the (1 x 3) RHEED pattern is observed. A c(2 x 10) structure has been proposed for the surface displaying the (1 x 5) diffraction pattern [3]. This structural model

is controversial, since it does not obey the electron counting rule, which has been a governing theorem to evaluate the plausibility compound semiconductor surface structural models. Moreover, authors from a theoretical investigation authors have evaluated the different models for the GaSb(001) surface reconstructions and have dismissed the c(2 x 10) model based on their *ab initio* total energy calculations [4].

In light of the ongoing debate over the GaSb(001) surface structures we have applied the surface x-ray diffraction technique to investigate the aforementioned surface phases. In addition to using SPring-8's superior x-ray beam characteristics, our study has the advantage that the measurement is carried out in situ, under technologically relevant conditions. Whereas the aforementioned STM measurements are performed at room temperature on a quenched surface, we measure the diffraction pattern, at elevated temperature and under a Sb flux of 0.25 ML/s.

The (1 x 5), and (1 x 3) surface phases were measured in succession on the same substrate. For both surfaces we collected a wide range of in-plane surface reflections, as well as several fractional order and integer-order crystal truncation rods. The in-plane data is used to determine the 2D atomic arrangement on the surface and the crystal truncation rods contain information from the 2D structure as well as the surface relaxations and registration of the surface reconstruction with the substrate. Standard correction factors have been applied to the data, including polarization, sample area, and geometrical corrections. The in-plane data was measured at H and K coordinates in all four quadrants of reciprocal space. The structure factors were averaged and the error bars were determined from a combination of systematic and statistical error. An agreement factor of 8% was determined for the data. The resulting in-plane structure factor maps measured at a constant L = 0.04 are displayed in figures 1 and 2.

We are performing structural analysis using standard techniques by fitting the data to the existing structural models documented in the literature. The superior quality of the data will

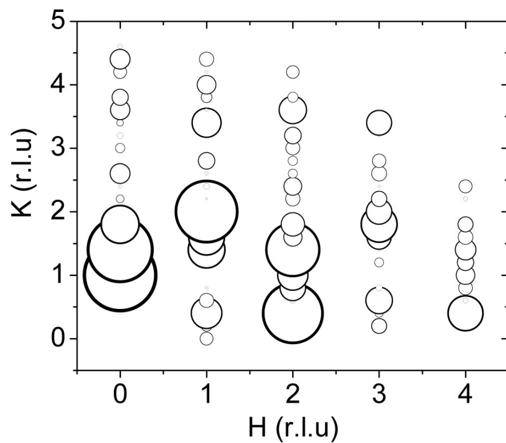

Figure 1. Symmetry averaged structure factors measured from the (1 x 5) reconstruction. The circumferences of the circles are proportional to the measured structure factors. L = 0.04.

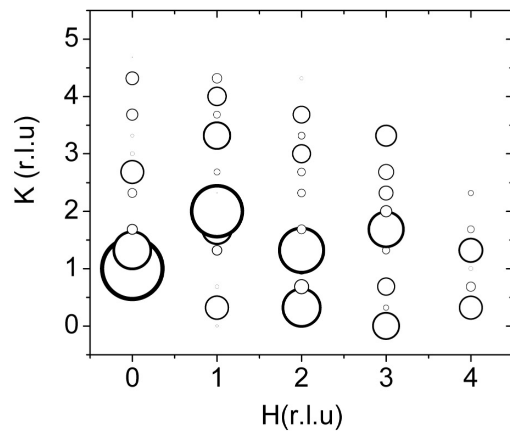

Figure 2. Symmetry averaged structure factors measured from the (1 x 3) surface reconstruction. The circumferences of the circles are proportional to the measured structure factors. L = 0.

enable us in parallel to apply more advanced analysis techniques, such as direct methods, that can produce directly and model independently the electron density on the surface. It is foreseeable at this point that the data acquired during this measurement will appear in two separate refereed journal articles.

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