Structural analysis of the BeTe(001) surface

C. Kumpf, A. Müller, W. Weigand, J. Wagner,1 V. Wagner,1 L. Hansen,1 S. Gundel,1 J. Geurts,1 O. Bunk,2 F. Wu,3 R. L. Johnson,3 and E. Umbach.

Experimentelle Physik II, Universität Würzburg, D-97074 Würzburg, Germany,
1 Experimentelle Physik III, Universität Würzburg, D-97074 Würzburg, Germany,
2 Materials Research Department, Risø National Laboratory, DK-4000 Roskilde, Denmark,
3 Institut für Experimentalphysik, Universität Hamburg, D-22761 Hamburg, Germany

Within the fabrication process of semiconductor-based electronic and optoelectronic devices the epitaxial growth behavior of thin films is crucial. In order to enable the possibility of designing the properties of the devices it is essential to gain full control over the growth behavior during the molecular beam epitaxy (MBE) process. This implies, that a detailed knowledge about the morphology and the geometric structure of surfaces and interfaces of the system is available. Among the II-VI compounds, BeTe provides unique opportunities, since it exhibits unusual electronic, vibrational and elastic properties, such as a very high band gap (4.2 eV), a high p-dopability, the lowest polarity of all II-VI compounds, a very high shear modulus and an extreme mass-asymmetry, leading to a very specific phonon dispersion behavior. Furthermore, the lattice mismatch to GaAs and ZnSe is very small, which allows high-quality epitaxial growth.

Here we report a detailed atomic model for the Te-rich BeTe(001)-(2×1) surface based on SXRD. The samples were prepared at Würzburg University in a Riber MBE System using standard techniques. A 25 nm thick BeTe layer was deposited at a substrate temperature of 350°C on undoped GaAs substrate, followed by two layers of amorphous Te and Se, 50 nm each, protecting the sample during the transport to HASYLAB. Desorption of the protective layers under LEED control recovered a sharp (2×1) reconstruction. Afterwards the samples were transferred to a portable UHV chamber, mounted on the z-axis diffractometer at the BW2 beamline, and a full-size data set was measured at a wavelength of 1.305 Å. The diffraction pattern revealed a p2mm symmetry. After a standard treatment of the raw-data the final data sets consisted of 28 independent in-plane reflections and eight fractional-order rods with 258 reflections. Crystal truncation rods were measured as well but not used for the refinement for reasons described elsewhere [1].

An extended fitting procedure yielded $\chi^2 = 1.14$ for the best fit. This was achieved using a parameter set containing the positions of the Te-dimer and three BeTe bulk-bilayers (14 positional parameters) and only three different Debye-Waller factors, one for the Te-dimer and one for each sort of atoms in the uppermost BeTe bilayer. The data and the corresponding atomic model is shown in Fig. 1. It should be noted, that it was necessary to use Keating-energy constraints [2] in order to achieve reasonable positions for the Be atoms. Due to their small atomic scattering factor their positions would be very unstable without these constraints.

The dominant structural feature of the Te rich BeTe(001)-(2×1) surface are Te-dimers on top of the surface which arrange themselves in one-dimensional rows. The dimer distance found in the SXRD experiment is 2.796(6) Å, a value which is in very good agreement with twice the covalent radius of Te (2.80 Å). Another important feature of the structure is a huge vertical buckling of the Te atoms in the uppermost bulk-like layer. The SXRD refinement yielded a height difference of $\Delta = 0.395(9)$ Å between the atoms Te-1 and Te-2 (see Fig. 1). The interaction between the buckling effect in the first bulk-layer and the dimerization in the ad-layer is mediated by the Be-1 atoms lying between the Te dimers and the Te-2 atoms. These atoms show a lateral relaxation of 0.16 Å in the direction towards the center of the unit cell. These strain-induced relaxation effects proceed into deeper layers with a decreasing amplitude, they can still be detected in the third Te bulk-layer. Small arrows in Fig. 1d illustrate the situation: The atoms of subsequent BeTe-bilayers are shifted alternatingly in lateral and vertical direction. In that way the strain induced by the surface dimers is effectively compensated in the uppermost three bulk layers.
Figure 1: SXRD Data and structural model for the BeTe(001)-(2\times1) surface. (a) Plot of the in-plane data. The areas of the open and filled semicircles represent measured (error bars shown by two semicircles) and calculated intensities, respectively. Gray/white circles have been scaled by a factor of 0.5 with respect to the black/white circles. (b) Fractional order rods. The model used for the calculations is shown from above (c) and from the side (d). In (c) the (2\times1) unit cell is indicated by a gray area. Small arrows in (d) indicate the direction of the relaxation of the atoms.

It can be speculated that the lateral relaxation of the Be-1 atoms is the reason for the linear arrangement of the Te-dimer rows which causes the (2\times1) superstructure cell. An alternative formation of a c(2\times2) superstructure consisting of alternating dimers, in which every second dimer in the row would be shifted by half of the unit cell in [1\bar{1}0] bulk-direction, would inhibit any lateral relaxation of the Be-1 atoms due to the c2mm-symmetry of that unit cell. (In a c(2\times2) unit cell the Be-1 atoms lie on the intersection point of two glide planes). As a consequence the buckling of the Te-2 and 3 atoms would be inhibited as well, i.e., the upper bulk layers would not be able to accommodate for any strain from the dimerized adlayer.

Finally it should be mentioned, that the BeTe(001)-(2\times1) model presented here is in extraordinary good agreement with results from Raman spectroscopy and density functional theory [1], which strongly supports its correctness.

References
