ZnS deposition onto bare and GaSe terminated Silicon-(111)-surfaces

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ZnS deposition onto bare and GaSe terminated Silicon-(111)-surfaces

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Abstract. The electronic properties and growth morphology of Si(111)/ZnS heterostructure modified by a GaSe van der Waals termination layer, which provides a chemical and an electronic passivation of the Si(111)-surface is investigated by surface sensitive methods (STM, LEED and SXPS). The van der Waals termination layer suppresses the Si-S interface reaction, which is observed for non terminated substrates. The interface electronic properties are nearly unchanged, but the morphology of the growing ZnS-film is dramatically changed. With the passivation layer ZnS grows as orientated pyramides with a (111) base area surface orientaion and (100)-facets. The sticking coefficient is reduced by a factor of ≈10 compared to bare Si(111), where ZnS grows as an untextured polycrystalline layer.

INTRODUCTION

The interface formation of silicon, as the base material of microelectronics and optically active compound II-VI-semiconductors is an ongoing research subject in semiconductor science and technology. The use of buffer and passivation layers between lattice mismatched 3-Dim materials is also important for controlling surface reaction and growth morphology. A GaSe passivation layer is used in this study as passivation layer, which provides a van der Waals type surface and saturates all dangling bonds of the Si(111)-surface [1, 2, 3, 4, 5]. This leads to a very stable chemical passivation of the Si(111) surface. Additionally the GaSe van der Waals termination leads to an almost ideal electronic passivation of the silicon surface states with almost flatband conditions. In this study the growth and interface properties of ZnS on the GaSe passivated surface is compared with the bare Si(111)-7x7 surface. The used silicon substrates were moderately (p- and n-type) doped.

EXPERIMENTAL RESULTS

The Si(111)-7x7 and the Si(111):GaSe-1x1 surfaces were prepared as published elsewhere [6, 7]. ZnS was successive deposited onto both surfaces at 150°C substrate temperature. The STM and LEED results were obtained at DAISY-FUN in Darmstadt [4]. For the SXPS investigations at BESSY II we used p-type samples with a misorientation of approximately 10° (highly stepped surface). The presented STM and LEED data results from n-type samples with a low misorientation of about 1°, with similar results obtained on p-type samples.

The SXPS results (p-type substrate) of bare and GaSe terminated Si(111) are shown in Fig. 1 and Fig. 2 left. With ZnS deposition onto Si(111)-7x7 the Si 2p line shows a broad chemically shifted extra emission on the high binding energy side. The spectra have been fitted with five components as shown in Fig. 1 middle. The components are derived from one Si 2p bulk emission and four different Si-S_x-bonds (x=1-4δ). The four Si-S components show a constant energy shift of δ=0.62±0.05 eV [8, 9]. The Si-S components and the stronger increase of the S-intensity in comparison to Zn indicates the formation of a S termination layer between Si and ZnS. The main Si-S component is shifted 3δ corresponding to three bonds of Si to S and corresponding to an 'on-top' position of the sulfur. S is also found on bridge-sites as an intermediate stage (1δ) [10]. This finding is also supported by the fact that Zn is not stable on the Si(111) surface and desorbs completely at temperatures of 100 to 200°C [11].

From the Si 2p-bulk component, the Zn 3d and S 2p binding energies and the difference between the valence band maximum (VBM) and the core level emission lines (Si=98,85eV [12]; ZnS (determined from a thick ZnS-layer): Zn=8.58 eV and S=159.99 eV) the presented VBM-positions (see Fig. 1) can be calculated. A valence band offset ΔE_{VB} of 1.2 eV and a conduction band offset ΔE_{CB} of 1.38 eV can be determined with the use of the bulk bandgaps of silicon and ZnS. This leads to a interface dipole potential of 1.21 eV, which is probably produced by the contact forming sulfur-layer. The result of the ZnS deposition on the GaSe passivated sur-

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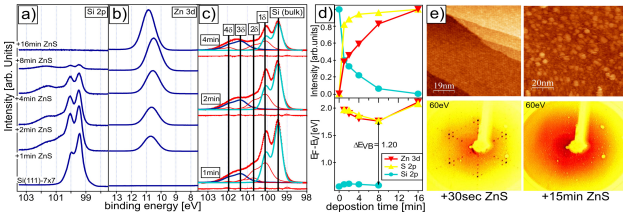

FIGURE 1. Results of ZnS-deposition onto the Si(111)-7x7 surface. a) Si 2p and b) Zn 3d-spectra ($h\nu = 240eV$); c) fitted Si 2p spectra with 5 components; d) intensity and VBM positions referred to the Fermi level are determined form the spectra a) and b); e) corresponding STM and LEED images.

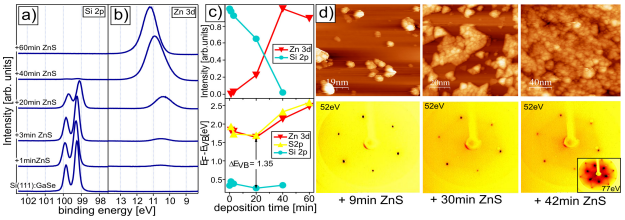

FIGURE 2. Results of ZnS-deposition onto the GaSe passivated Si(111)-1x1 surface. a) Si 2p and b) Zn 3d-spectra ($h\nu = 240eV$); c) intensity and VBM positions are determined form the spectra a) and b); d) corresponding STM and LEED images.

face are shown in the left part of Fig. 2. The Si, Zn and Se show a one component spectrum and the resulting VBM positions and intensities are also given. No interface reaction could be detected with the GaSe passivation layer. From the evolution of the VBM energies ΔE_{VB}=1.35 eV, ΔE_{CB}=1.23 and a dipole δ=0.62 eV were evaluated. The deduced band offsets are very similar for both surfaces. The different interface dipoles result from the fact, that the GaSe half-sheet produces a surface dipole in the range of 0.45 eV [5]. The electronic properties of Si(111):ZnS and Si(111)GaSe:ZnS are very similar.

But with only a small difference of the band offsets (0.15 eV) the surface morphology is dramatically changed (see STM and LEED-images in Fig. 1 and 2). ZnS grows layer-by-layer on the Si(111)-7x7 surface with no long range in the LEED-images as also evident from the SXPS intensities. ZnS first starts to grow only at step-edges and defects on the Si(111):GaSe surface (see Fig. 2 STM-images after 9min). With longer deposition time the clusters get a triangular shape and they form pyramides with (100)-facets, as derived from additional LEED reflexes (see LEED-pattern after 42min). The ZnS-pyramides grow epitaxial onto the GaSe passivated surface. The non-exponential decay of the XPS intensities also indicates a cluster growth. Zn is probably situated at the base layer of the pyramides because of its possibility to interact with the double filled electron orbital of the selenium from the passivation layer.

CONCLUSION

The electronic properties of the ZnS-Si interface are not (or only lightly) changed by the GaSe half-sheet passivation layer. Morphology, crystallinity and sticking coefficient are modified dramatically. The GaSe half-sheet leads to the formation of ZnS pyramides which are orientated to the substrate. The sticking coefficient is reduced by a factor of ten, which can be used for the local deposition of ZnS on non passivated areas. This may be useful for the manufacturing of ZnS-quantumdots and ZnS-quantumwires on Si(111).

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REFERENCES

1. Koebel, A., Zengh, Y., Petroff, J., Boulliard, J., Capelle, B., and Eddrief, M., *Physical Review B*, **56**, 12296–12302 (1997).
2. Meng, S., Schroeder, B. R., Bostwick, A., and Olmstead, M. A., *Physical Review B*, **64**, 235314–1–8 (2001).
3. Meng, S., Schroeder, B. R., and Olmstead, M. A., *Physical review B*, **61**, 7215–7218 (2000).
4. Fritsche, R., Wisotzki, E., Thißen, A., Islam, A. B. M. O., Klein, A., Jaegermann, W., Rudolf, R., Tonti, D., and Pettenkofer, C., *Surface Science*, **515**, 296–304 (2002).
5. Fritsche, R., Wisotzki, E., Islam, A. B. M. O., Thißen, A., Klein, A., Jaegermann, W., Rudolph, R., Tonti, D., and Pettenkofer, C., *Applied Physical letters*, **80**, 1388–1390 (2002).
6. Ohta, T., Klust, A., Adams, J., Yu, Q., Olmstead, M., and Ohuchi, F., *Physical Review B*, **69**, 125322 (2004).
7. Jaeckel, B., Fritsche, R., Klein, A., and Jaegermann, W., *Physical Review B*, **submitted** (2004).
8. Weser, T., Bogen, A., Konrad, B., Schnell, R. D., Schug, C. A., and Steinmann, W., *Proceedings of the 18th International Conference on the Physics of Semiconductors*, pp. 97–100 (1987).
9. Hunger, R., Pettenkofer, C., and Scheer, R., *Journal of Applied Physics*, **91**, 6560–6570 (2002).
10. Papageorgopoulos, A. C., and Kamaratos, M., *Surface Science*, **504**, L191–L195 (2002).
11. Lifshits, V. G., Saranin, A. A., and Zotov, A. V., *Surface phases on Silicon*, John Wiley & Sons, Chchester, New York, Brisbane, Toronto, Singapore, 1994.
12. Himpsel, F. J., Hollinger, G., and A., P. R., *Physical Review B*, **28**, 7014–7018 (1983).