

The bonding configuration of Cyclopentene and 1,4-Cyclohexadiene on GaAs(001) surfaces

R. Paßmann^{1,2}, T. Bruhn², C. Friedrich², G. Gavrila³, D. R. T. Zahn³, W. Braun⁴,
W. Richter^{2,5}, N. Esser^{1,2}, P. Vogt²

¹ISAS – Institute for Analytical Sciences – Department Berlin, Albert-Einstein- Str. 9, 12489 Berlin, Germany

²Institute of Solide State Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

³Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

⁴BESSY GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany

⁵Universita degli Studi Roma “Tor Vergata”, Via della Ricerca Scientifica 1, 00133 Roma, Italy

During the last year we investigated the adsorption and bonding configuration of Cyclopentene (C_5H_8) and 1,4-Cyclohexadiene (C_6H_8) on InP(001) and the c(4x4), (2x4) and (4x2) surface reconstructions of the GaAs(001) surface. Our aim was to obtain information which helps to elucidate the important role of the surface dimer configuration and the influence of the number of double bonds within organic hydrocarbon ring molecules on the interface formation. Yet, no comprehensive study of these parameters on the important organic/inorganic interfaces can be found in literature and most of the work available was obtained on Si(001)(2x1) surfaces. On the other hand III-V (001) semiconductor surfaces exhibit the potential of different surface stoichiometries with different atomic surface structure (i.e. dimer structure) and different electronic and optical properties. In this report we will focus on the results concerning GaAs(001). Here, we could demonstrate that the surface dimer structure indeed influences the bonding configuration of 1,4-cyclohexadiene and Cyclopentene on GaAs(001) significantly. These results are also important for an understanding of the interface formation between organic molecules and semiconductor surfaces in general. In order to clarify the chemical composition and surface bonding sites for the molecules on the different surfaces SXPS measurements were carried out at the PM-RD and PM3 beamlines at BESSY.

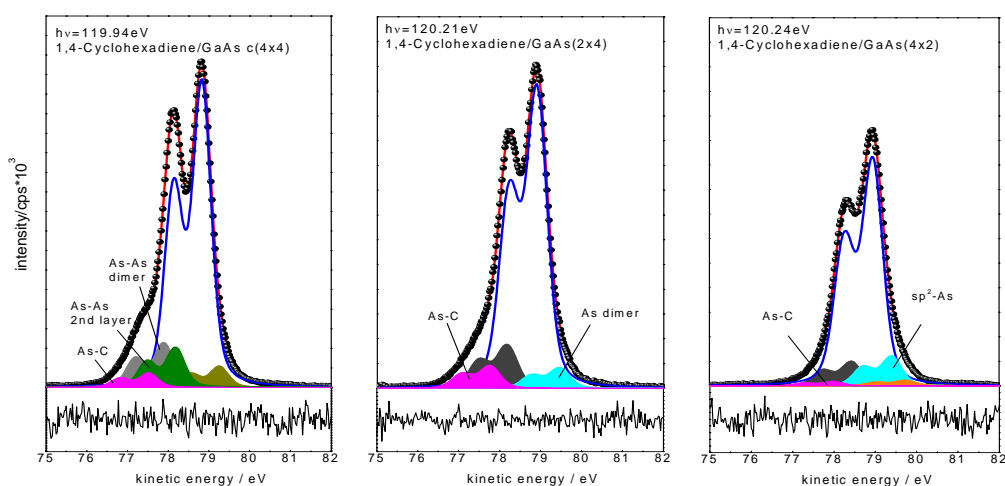


Fig.1: Core-level of As3d for the with 1,4-Cyclohexadiene saturated GaAs(001)c(4x4) on the left, (2x4) middle and (4x2) on the right, respectively.

1,4-Cyclohexadiene adsorption on GaAs(001) surfaces

After the deposition of 1,4-Cyclohexadiene the saturated surface was characterized by SXPS. The line shape of the clean core level is comparable to previous work. The As3d core level are depicted in Fig 1. An additional component (As-C) was observed

for all three surfaces at the lower kinetic energy side with respect to the bulk component. It is reasonable to conclude that this component can be assigned to As-atoms which are bonded to C-atoms from the Cyclopentene molecules. Within the Ga3d core level emission line no additional components can be observed.

The analysis of the C1s core levels for the three GaAs(001) surfaces saturated with 1,4-Cyclohexadiene is shown in Fig. 2.

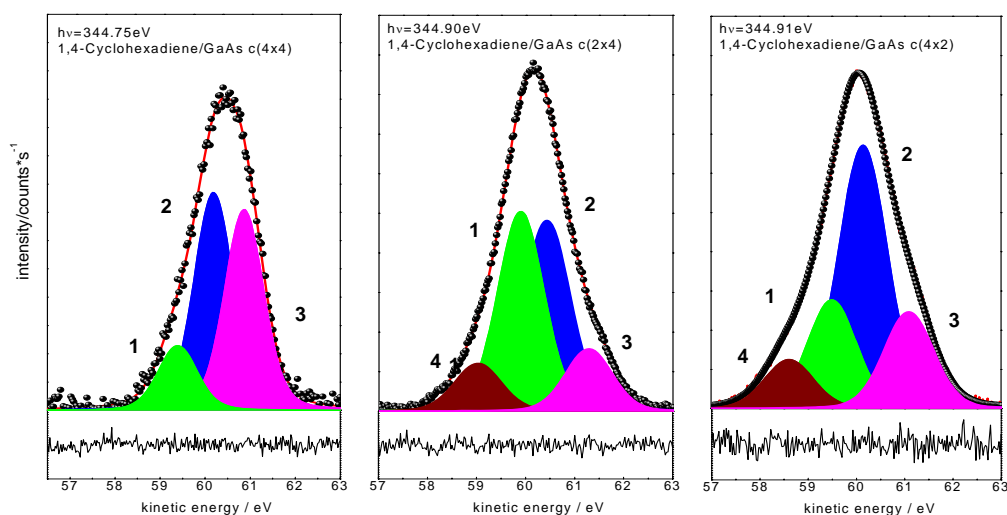


Fig.2: Core-level of C1s for the with 1,4-Cyclohexadiene saturated GaAs(001)c(4x4) on the left, (2x4) middle and (4x2) on the right, respectively.

In all three cases three main components within the C1s line shape are found by numerical analysis and a fourth one for the (2x4) and (4x2) reconstructed surfaces. The component 1 can be related to electrons which are included in the carbon-carbon double bond and the component 2 is related to the electrons of carbon atoms which are involved in the single carbon-carbon bond. The component labelled with 3 and 4 for the (2x4) and (4x2) reconstructed surfaces can be assigned to the electrons of the carbon atoms which are involved in the C-As bondings to the first and second layer As-atoms. Therefrom we can conclude that the 1,4-Cyclohexadiene molecules bonds to the topmost As-atoms of each surface reconstruction. In all three cases it is obvious that beside the chemisorption also physisorption is found indicated by component (1) which is related to electrons of the C=C double bond. This component is very pronounced for the (2x4) reconstructed surface indicating more carbon double bonds and thus more 1,4-Cyclohexadiene molecules which stay intact on this surface after deposition. This is a hint towards a physisorption on the (2x4). For the c(4x4) and (4x2) this component is not as pronounced as for the (2x4).

Cyclopentene adsorption on GaAs(001) surfaces

An additional component was also found in the core level line shape of the As3d emission. No additional component appeared in the numerical analysis for Ga3d. The C1s core level spectra of Cyclopentene adsorbed on the GaAs(001) surfaces are shown in Fig. 3. Also for each surface reconstruction the core levels were fitted with three components with numerical analysis similar as for the adsorption of 1,4-Cyclohexadiene while for the (4x2) four components were necessary. Again for each reconstruction the component 3 was observed which is related to the electrons in an As-C bond.

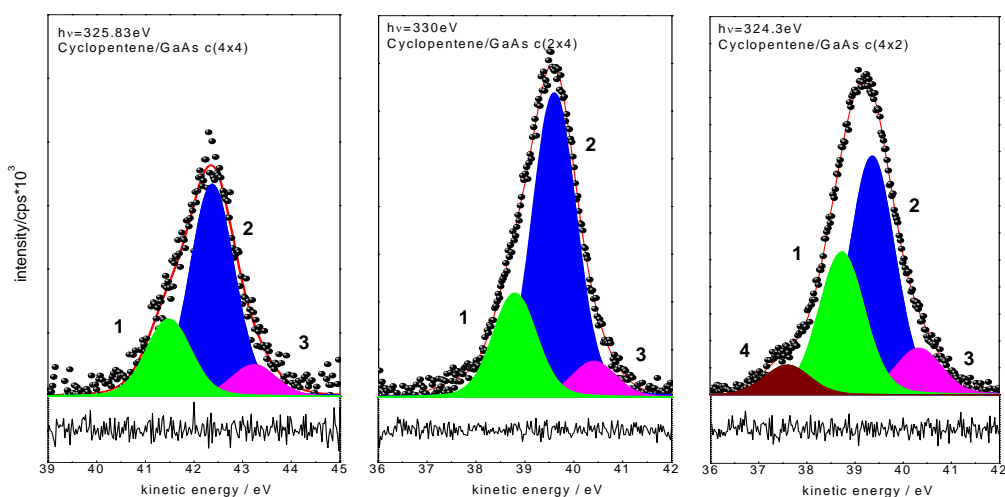


Fig.3: Core-level of C1s for the with Cyclopentene saturated GaAs(001)c(4x4) on the left, (2x4) middle and (4x2) on the right, respectively.

The additional component 4 for the (4x2) reconstructed surface indicates bonding not only to the topmost As atoms but also to the second layer As atoms as in the case of 1,4-Cyclohexadiene. Component 1 should not appear in case of Cyclopentene because if the molecule bonds covalently to the surface the double bond should be broken. Therefrom we can conclude that besides the chemisorption also a physisorption of the molecules takes place.

Summary and conclusion

For both molecules it can be concluded that the molecules chemisorb but also physisorb on the surfaces. In all cases a new component appears only in the As3d core level line shape and no additional component for the Ga3d core level was found. Therefrom we can conclude that it is much more attractive for the hydrocarbon ring molecules to form a bond to the filled dangling bonds of the topmost As-atoms than to the Ga-atoms. The amount of additionally physisorbed molecules is different for each surface reconstruction. In the case of 1,4-Cyclohexadiene it is also difficult to distinguish between chemisorption and the additional C=C bond within the organic molecule. It can be concluded that both molecules interact with their C=C double bond and the surface topmost As-atoms. This last finding is important since the gallium-atoms/dimers seem to play no role in the interface formation in these cases. Furthermore it should be pointed out that the organic hydrocarbon ring molecules used in this work do not destroy the surface reconstruction and form an atomically abrupt interface. The molecules can be thermally removed by annealing and a clean well reconstructed GaAs(001) surface is formed again as verified by SXPS and RAS. Our SXPS results are supported by RAS measurements [4] and STM results.

We would like to acknowledge financial support by the BMBF under grant number – MUSTANG BMBF 05 KS40C1/3.

References

- [1] W. G. Schmidt, F. Bechstedt, W. Lu, J. Bernholc, Phys. Rev. B 66, 085334 (2002), [2] W. G. Schmidt, F. Bechstedt, K. Fleischer, C. Cobet, N. Esser, W. Richter, J. Bernholc, G. Onida, Phy. Stat. Sol (a) 188, 1401 (2001), [3] W. G. Schmidt, N. Esser, A. M. Frisch, P. Vogt, J. Bernholc, F. Bechstedt, M. Zorn, T. Hannappel, S. Visbeck, F. Willig, W. Richter, Phys. Rev. B 61, R16335 (2000), [4] R. Passmann, M. Kropp, T. Bruhn, B.O. Fimland, F. L. Bloom, A. C. Gossard, W. Richter, N. Esser, P. Vogt, Applied Physics A, in print (2007).