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Si *2p* core levels – a fingerprint of the π electrons in epitaxial silicene

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Introduction

While the recently discovered epitaxial silicene is the Si analogue of epitaxial graphene, its structural and electronic properties are considered to be distinct from those of his cousin [1,2]. As we have reported in our previous PF report (18A/2010G571) for silicene on ZrB$_2$(0001) thin films, atomic-scale buckling is associated with a variation of the sp^2/sp^3 ratio in between the three chemically distinguishable atoms which in turn leads to chemical shifts visible in the Si *2p* core levels energies [1]. On the other hand, the electronic structure and also the final state screening response may be affected by the close contact of silicene with the metallic substrate.

Experimental

High-resolution, Si *2p* core-level photoelectron spectra of epitaxial silicene on ZrB$_2$(0001) thin films prepared on Si wafers have been obtained with the SCIENTA SES200 analyzer at BL13A using three different photon energies. The normal emission geometry has been employed.

Results

The normal emission Si *2p* photoelectron spectra obtained with photon energies of 130, 340 and 700 eV are shown in Figure 1. For 130 eV, the spectrum of the doublet resembles the one reported previously [1]. Owing to the higher resolution, however, for both the $2p_{1/2}$ and $2p_{3/2}$ lines, two peaks are well separated from each other. As compared to the binding energy of the bulk component in sp^3-hybridized silicon [3], binding energies in silicene are 200 - 460 meV lower. This is consistent with the occurrence of an efficient core-level screening due to the presence of the low-energy π-electronic valence band structure resulting from a large degree of sp^2 hybridization.

In the spectrum obtained with the photon energy, $h\nu$, of 700 eV, at the high-energy side of the spectrum, the tail structures gains spectral weight and becomes even structured. An enhancement of spectral intensity is found in two groups of features that are split by 0.6-0.7 eV. Note that within the uncertainty of the evaluation, the splitting follows the spin-orbit splitting such that these two features may be attributed to shake-ups associated with the $2p_{3/2}$ and $2p_{1/2}$ main lines, respectively. These shake-up features, denoted s_1, s_2, s_3 and s_4, are observed at a binding energy approximately 1.95 eV higher than the main peaks. This energy is close to the prominent peak at 1.7 eV in the calculated optical absorbance that is related to the predicted high optical transition strength between π bands at the *M* point of non-reconstructed, free-standing silicene [4]. In order to allow for this good agreement, the substrate must exert only a minor influence on the π bands at energies away from the Fermi level.

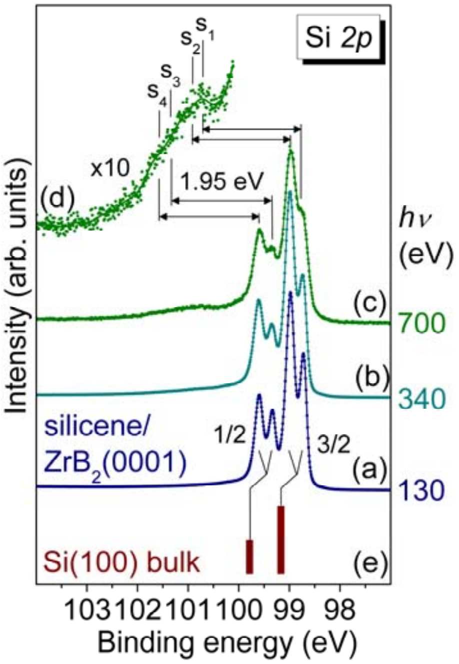

Fig. 1: Normal-emission Si *2p* photoelectron spectra of silicene on a thin ZrB$_2$(0001) film obtained at (a) $h\nu$ = 130 eV, (b) 340 eV, and (c) 700 eV. (d) Magnification of the spectrum plotted as (c). (e) The binding energies of Si atoms in the bulk of *sp^3*-hybridized silicon single crystals [3].

References

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