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Detecting the parity of electron wave functions in solids by quantum-well states of overlayers

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Abstract. We present an approach to monitor the parity of wave functions of electronic states of bulk solids, which was elaborated on the model Ag/W(110) system. The dispersion of quantum-well (QW) states formed in the thin Ag layer was examined by means of angle-resolved photoemission. The obtained experimental data were compared with results of layer Korringa–Kohn–Rostoker calculations. We found that around **k** points, where the two-dimensional QW bands cross the projected bulk bands of the W substrate of the same symmetry, broad hybridization gaps in the QW distributions are observed. Careful analysis based on a symmetry approach for the electronic bands in the Ag monolayer and the W substrate suggests that respective gaps may generally be taken as a fingerprint for the interaction with substrate states of *even* parity with respect to the emission plane. We anticipate that QW states may be used as a probe for symmetry properties of strongly correlated states in systems like heavy-fermion compounds that are difficult to access theoretically within an *ab initio* approach.

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Contents

1. Introduction

Experimental and theoretical studies demonstrate that the parity of wave functions of electronic states governs many phenomena in strongly correlated electron systems [1] and provides a key for a deeper understanding of such effects as, for example, heavy-fermion behaviour [2, 3]. At the same time information on the parity of wave functions of electronic states in these systems is hardly available from theoretical approaches, but highly motivated and strongly desirable for a careful and reliable interpretation of such phenomena. In order to gain experimental insight into the symmetry properties of electronic states in solids we draw attention to the phenomenon of quantum wells (QW) in thin overlayers of metals. QW states in metallic nanostructures have already been objects of continued interest for more than 20 years, nevertheless, they exhibit permanently novel fascinating phenomena. In the case of a thin film, the physical origin of the formation of the QW states is the confinement of electrons by potential barriers at the surface and the interface. The latter can be induced by energy or symmetry gaps of the substrate. As a consequence, the dispersion of the energy band being continuous in the bulk of the crystal breaks up into discrete energy states $E(\mathbf{k}_\perp)$ for the momentum direction perpendicular to the surface of the thin film. These discrete QW states can be probed by angle-resolved photoemission spectroscopy (ARPES) [4]. Parallel to the surface, electrons experience a periodic potential, therefore the band structure consists of a set of so-called QW subbands. These subbands reveal an almost two-dimensional behaviour that may, however, be affected dramatically by interactions with three-dimensional bands of the substrate.

Recently, it has been shown that the continuous dispersion of QW subbands breaks up near the edges of projected bulk bands of the supporting material [5]–[8] and in this way permits insight into ground-state properties of the substrate. In particular, such unusual dispersion of QW subbands was experimentally observed for the Ag/Ge(111) system and explained in terms of many body interactions [6]. Later on, it was established that in a Cu/Co/Cu(001) magnetic multilayer structure [7] penetration of the sp-like QW state from the non-magnetic Cu layer into the Co barrier layer and its coupling with Co minority states leads to non free-electron-like dispersion of quantized states, too. This offers an intriguing opportunity to tune the strength of electron coupling in magnetic multilayer structures [7]. Lately, it was shown in [9] that the energy dependence of the phase of QW states can be used as an elegant instrument to probe electronic bands of underlying materials. This indirect possibility to explore electronic properties applying QW states is of decisive importance for correlated systems, where direct

photoemission (PE) excitation leads to final states that are very different as compared to the initial states.

Basically, experimental studies of QW states in thin layers of simple metals like Au, Ag, Mg, Al, etc, offer an interesting opportunity: deposition of a thin layer of appropriate material onto the surface of the studied strong correlated system leads to the appearance of QW states within the layer with particular (s-, p- or even d-) angular-momentum character. Then, possible deviations from a monotonic dispersion of the two-dimensional QW bands and, in particular, the appearance of gaps indicates a coupling between QW- and substrate bands with wave functions of the same parity. Since the symmetry properties of two-dimensional QW bands can be determined easily, they may be used successfully as fingerprints to probe the parity of substrate bands. Note that the parity data provide information about site-specific localization of electron densities that may be directly used, e.g. to understand interactions in correlated materials like heavy-fermion systems (f–d hybridization).

However, a detailed experimental analysis of subband dispersion requires that the QW states of the overlayer are unambiguously related to the thickness of the film, or in other words should be atomic-layer resolved. Otherwise the subbands represent bunches of components corresponding to different thicknesses of the film [6].

Therefore, we chose the Ag/W(110) system for our experiments, which represents in this respect an ideal candidate for studying coupling phenomena between substrate and overlayer states. It was demonstrated that deposition of thin layers of Ag metal on W(110) leads to formation of atomic-layer resolved QW states in a wide **k** and energy range [10, 11] that gives the opportunity to explore their subbands structure with ARPES. Moreover, this system was studied carefully by means of scanning tunnelling microscopy (STM) [12]. The obtained STM data can be used for a proper structure model necessary for a quantitative theoretical analysis. In the present paper, we demonstrate by means of an ARPES study of Ag/W(110) and layer Korringa–Kohn–Rostoker (LKKR) calculations that energy crossings of QW and some substrate energy bands lead to the formation of broad hybridization gaps around the **k** point of the crossings.

2. Experimental details

The ARPES experiments were performed using a photoelectron spectrometer equipped with a Scienta SES-200 hemispherical electron-energy analyser and a high-flux He-resonance lamp (Gammadata VUV-5010) in combination with a grating monochromator. All PE spectra were acquired at a photon energy $h\nu = 40.8\,\mathrm{eV}$ (He IIα) and room temperature with an angular resolution of 0.3° and a total-system energy resolution of 50 meV. Electron band dispersions were measured along the [001]-direction ($\overline{\Gamma}-\overline{\mathrm{H}}$) of the surface Brillouin zone (BZ) of W(110) by varying the polar emission angle. The samples were prepared *in situ* under ultra high vacuum conditions at a base pressure of 1×10^{-10} mbar. Thin films of Ag were deposited on a W(110) substrate kept at room temperature, with a deposition rate of $0.5\,\text{Å}\,\mathrm{min}^{-1}$ monitored by a quartz microbalance. The film thickness was crosschecked by the presence of layer-resolved QW states. Prior to film preparation, the substrate was carefully cleaned by repeated cycles of heating up to 1300 °C in oxygen atmosphere for 15 min each (with a partial pressure of 5×10^{-8} mbar) and subsequent flashing up to 2300 °C. The crystalline quality was monitored by low-energy electron diffraction and PE data gave no hints of chemical contaminations.

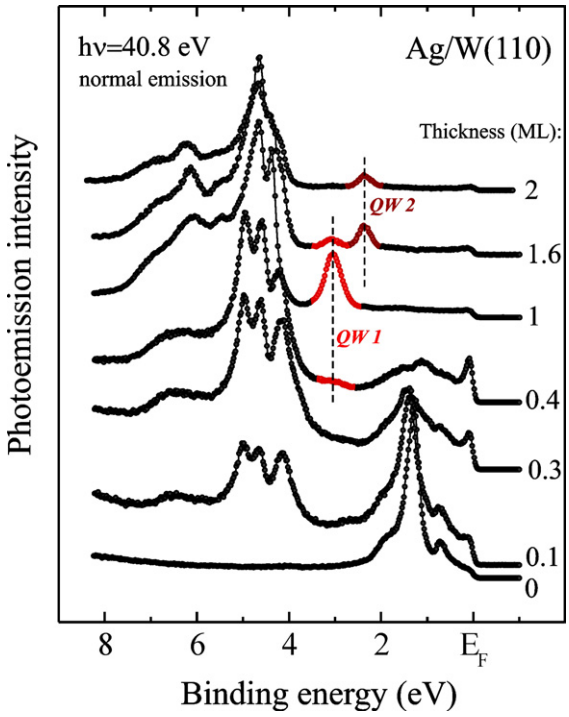

Figure 1. Experimental angle-resolved PE spectra taken in normal emission geometry from clean W(110) and Ag/W(110) at various coverages.

3. Experimental results

Angle-resolved PE spectra recorded in normal emission geometry from the clean W(110)-surface and after deposition of Ag films of various thicknesses are presented in figure 1. The strong electron emission signal from W 5d states observed around ∼1.5 eV binding energy (BE) is strongly suppressed upon silver deposition and completely disappears in the spectrum for the film thickness of about 1 monolayer (ML). This phenomenon is well known from, e.g. studies of rare-earth films on W(110), where even in case of monolayer coverage the substrate emission is almost completely quenched. However, quantitative theoretical description of this phenomenon is still lacking since the analysis of the respective interfaces by means of slab or LKKR approach demands the assumption of a well-defined periodicity of the whole system that is violated. The presence of an Ag overlayer is reflected by strong Ag 4d derived emission between 4 and 7 eV BE that are visible even at submonolayer coverage. With increasing amount of silver atoms on the surface the shape of the Ag 4d derived signal changes and approaches that of Ag metal at a coverage of about 2 ML. Of particular interest is the BE range of 0–4 eV. Here, it is possible to observe two distinct features at 3.2 and 2.4 eV BE, which represent QW states derived from the nearly-free-electron-like Ag sp band [10, 11]. Formation of these well-defined peaks indicates a smooth growth of silver overlayers in the monolayer regime with a roughness of the films of the order of one monolayer. This behaviour is in agreement with a recent STM study of Ag growth on W(110) [12]. Observation of atomic-layer resolved QW peaks offers the opportunity to explore the evolution of their dispersion. To this end, we performed careful band mapping of the clean W(110)-surface and Ag film of different coverages. In figure 2, we illustrate the results

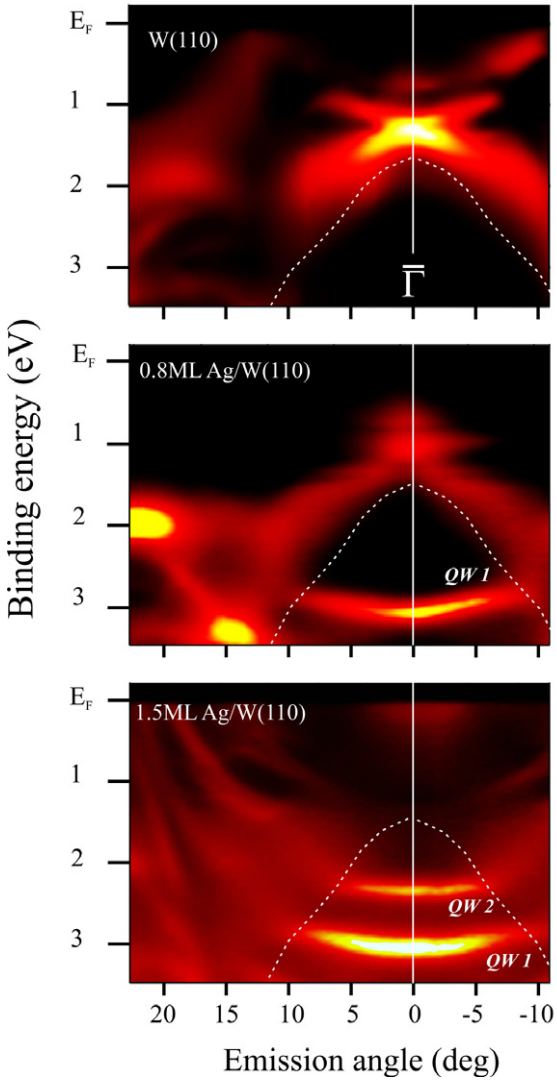

Figure 2. PE intensity distributions obtained along the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ direction of the surface BZ of clean W(110) (top panel) as well as ∼0.8 ML (middle) and 1.5 ML Ag/W(110) (bottom). PE intensities are plotted in a colour scale representation as a function of polar emission angle. Light colours denote high intensity while dark colours are used for low intensity regions. The dashed lines are guides to the eye to follow the area of a projected W(110) bulk bandgap.

of such two-dimensional band structure mapping obtained from the clean W(110)-surface (top panel) and after deposition of Ag metal of a nominal thickness ∼0.8 and 1.5 ML, respectively (middle and bottom panels). Inspecting the band topology of clean W(110), one observes a large bell-shaped energy gap around the $\overline{\Gamma}$ point. The border of this gap is marked in figure 2 by a dashed line. Upon deposition of silver onto the atomically clean W surface considerable changes in the band topology occur, and for a nominal thickness of about 0.8 ML (middle panel) one observes that the gap is filled with a free-electron-like parabolic band (*QW 1*) around the $\overline{\Gamma}$ point with a minimum at 3.2 eV BE. Upon further deposition of Ag, a second parabolic band

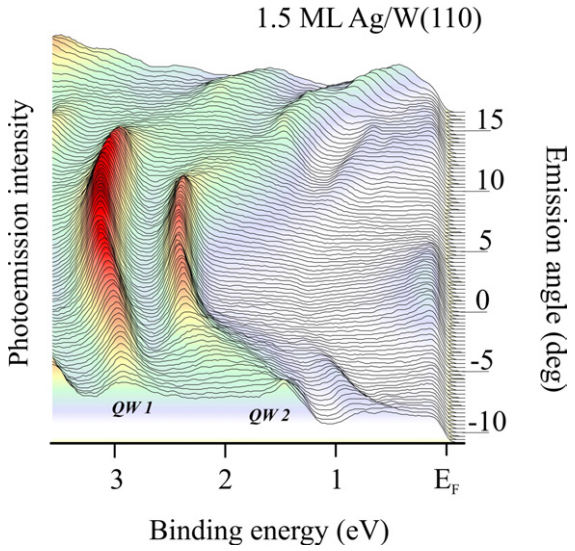

Figure 3. Series of angle-resolved PE spectra of ∼1.5 ML Ag/W(110) taken along the $\overline{\Gamma}$ – $\overline{\mathrm{H}}$ -direction of the surface BZ of W(110).

QW 2 fills the bell-shaped gap with a minimum at 2.4 eV BE. These new bands can readily be identified as QW subbands associated with film thickness of one and two silver monolayers, respectively.

Careful analysis of the Ag QW bands dispersion in figure 2 (bottom panel) reveals two observations: (i) outside the W(110) bandgap the intensity of the QW states drops, and (ii) the shape of the dispersion is not entirely parabolic but reveals gaps in the region of the W substrate band crossings. For a more pictorial view of this unusual behaviour, we present in figure 3 a series of angle-resolved PE spectra taken along the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ -direction of the surface BZ of W(110) for a coverage ∼1.5 ML.

In order to explore the dispersion and intensity behaviour in more detail, we concentrated on the region of the gaps and repeated measurements with enhanced angular resolution (up to 0.1°). For further analysis we chose the 1 ML Ag/W(110) system, since here only the *QW 1* subband is visible that simplifies the analysis. The obtained experimental results are presented in figure 4(a) in a three-dimensional plot of the PE signal as a function of polar emission angle and BE. The strong splitting and 'kink'-like behaviour of the *QW 1* subband near the W band edge is clearly visible.

4. Theoretical calculations

4.1. LKKR approach

In order to simulate the PE spectra, we have modelled the Ag overlayer in the following way: assuming that for 1 ML Ag most of the silver atoms still reside in or very near to tungsten bcc substrate positions [12], the substrate lattice was continued into the vacuum and the lattice sites closest to the W(110)-surface were occupied by Ag atoms. As a next step, the electronic structure of a slab of five W atomic layers covered on both sides by Ag monolayers was

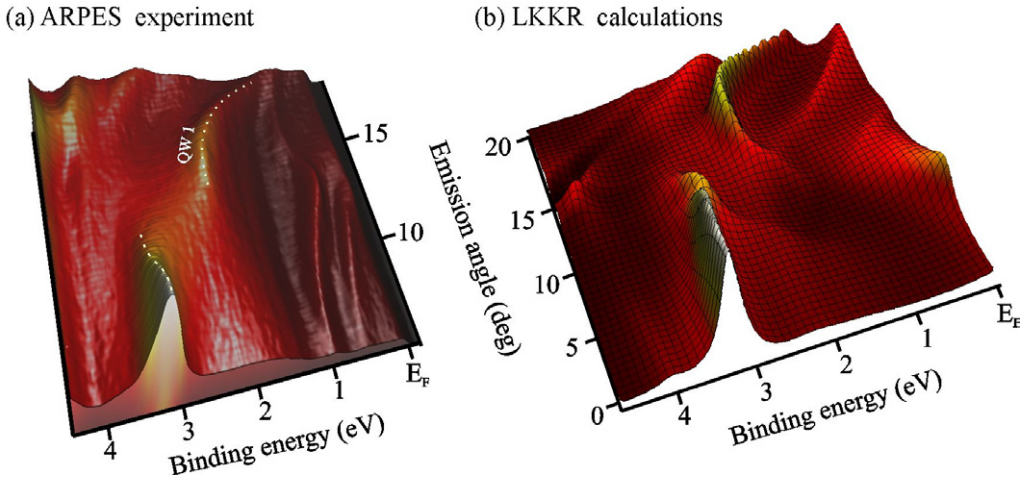

Figure 4. Three-dimensional presentation for 1 ML Ag/W(110) system of: (a) angle-resolved PE data acquired along the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ -direction in a proximity of the crossing of the *QW 1* subband and projected bulk bands of tungsten and (b) spectral function calculated by means of the LKKR method for $\mathbf{k}_{||}$ along $\overline{\Gamma}$–$\overline{\mathrm{H}}$ -direction.

calculated by means of a full-relativistic version [13] of the linear-muffin-tin-orbital (LMTO) method [14]. The calculated self-consistent potentials of Ag and different W atoms (that have different positions with respect to the surface) were then used for further calculations, performed by means of the LKKR approach [15] that realizes a relativistic one-step model to compute angle-resolved PE spectra. This basically *ab initio* approach contains, however, two adjustable parameters that influence the results of the calculation. One of them is the position of the surface barrier which can affect the energy position of surface states. In our calculation, this barrier was placed at 60% of the W interlayer distance above the Ag layer in order to shift the bottom of the Ag 5s-derived band to the energy position observed in the PE experiment. The second parameter is the imaginary part of the optical potential that describes the damping of the electron wave in the crystal. This quantity was chosen to be 1 eV for the Ag layer and 5 eV for the W substrate. The latter value seems to be quite large, since corresponding values for metals usually do not exceed 2 eV. However, only such a large value resulted in an intensity suppression of W-derived emissions in the calculated spectra to the same order of magnitude as those observed in the experimental data. A possible explanation for the (already mentioned above) strong damping of the W signal can be a slight mismatch between the Ag overlayer and the W substrate caused by the different radii of the involved atoms. Even small deviations the positions of the Ag atoms from their *assumed* sites will lead to an appearance of an imaginary component of the **k** vector of substrate Bloch functions resulting in a reduced intensity of their PE signal. As obvious from figure 4(b), the calculated results agree well with the experimental data. The main spectral feature is a parabolic-like band that has its maximum intensity at the $\overline{\Gamma}$ point and undergoes a splitting for polar emission angles between 10° and 15°. Unfortunately, the LKKR method does not allow us to assign the predicted spectral features to solid-state electron wave functions.

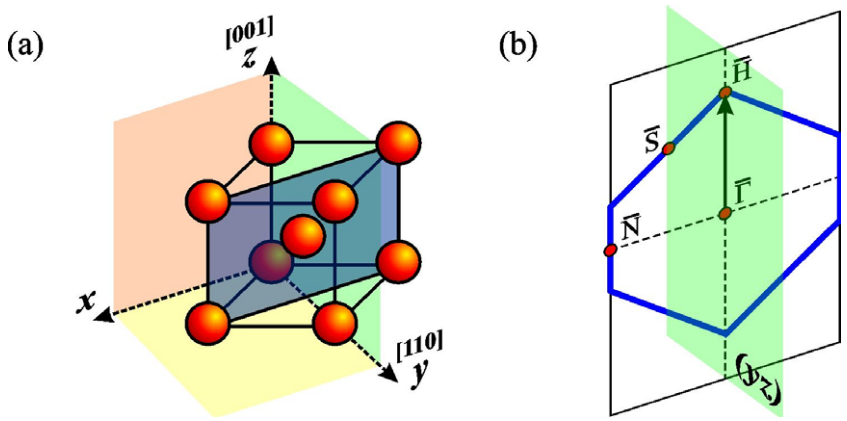

Figure 5. (a) Bulk unit cell of W with coordinate system used for symmetry analysis. (b) Geometry of the PE experiment in **k** space; escaping photoelectrons are measured in the (yz) plane probing the electron states along the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ -direction in the surface BZ.

4.2. Full-relativistic LMTO method

In order to analyse the electronic structure of the Ag/W(110) system in detail, we performed, therefore, full-relativistic LMTO calculations for a freestanding two-dimensional Ag monolayer and for a bulk W crystal. For the latter the resulting energy bands were projected onto the (110)-plane. In order to facilitate the wave function symmetry analysis, we introduce a coordinate system related to the geometry of the experiment (see figure 5). The z-axis is taken along the [001]-direction and the y-axis is normal to the (110)-plane. This definition is different from the coordinate system chosen usually for cubic lattices (with axes along the cube edges) by a rotation of 45° with respect to the z-axis.

Now, the (110)-surface is parallel to the (xz)-plane and emitted electrons are measured in the (yz)-*emission* plane. With these definitions *even* and *odd* parity functions with respect to the mirror (yz)-plane may easily be identified as $\Psi(-k_x, k_y, k_z) = \Psi(k_x, k_y, k_z)$ and $\Psi(-k_x, k_y, k_z) = -\Psi(k_x, k_y, k_z)$, respectively. Moreover, for the chosen geometry of the PE experiment, $k_x = 0$ (or, taking into account a finite angular resolution, k_x is very small) and the amplitude of the *odd* wave functions practically disappears suppressing strongly their contribution to the transition matrix elements. As a result, the measured PE intensity distribution reflects energy bands that are *even* with respect to the mirror (yz)-plane.

Figure 6(a) shows the calculated energy bands in the free-standing Ag monolayer along the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ -direction. Point $\overline{Z}$ denotes the midway of the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ distance. In the energy region between 3 eV BE and the Fermi level one observe a free-electron-like parabolic band that is formed mainly by Ag 5s-derived states. This band reaches the Fermi energy close to the $\overline{Z}$ point that is probed in our PE experiment at a polar emission angle of 19°. In the vicinity of the $\overline{\Gamma}$ point, the 5s states are hybridized with Ag 4d states (derived mainly from $d_{3z^2-r^2}$ orbitals). This modifies the shape of the free-electron-like band by increasing the effective electron mass in this **k** region. The contribution of the d states also increases the photoionization cross-section in this region and is responsible for the observed enhancement of emission intensity of the QW states around the $\overline{\Gamma}$ point. At 2 eV BE, the top of the energy band with a hole-like dispersion can be seen that is derived mainly from d_{xz} orbitals. Since the electron states of this band are *odd* with respect

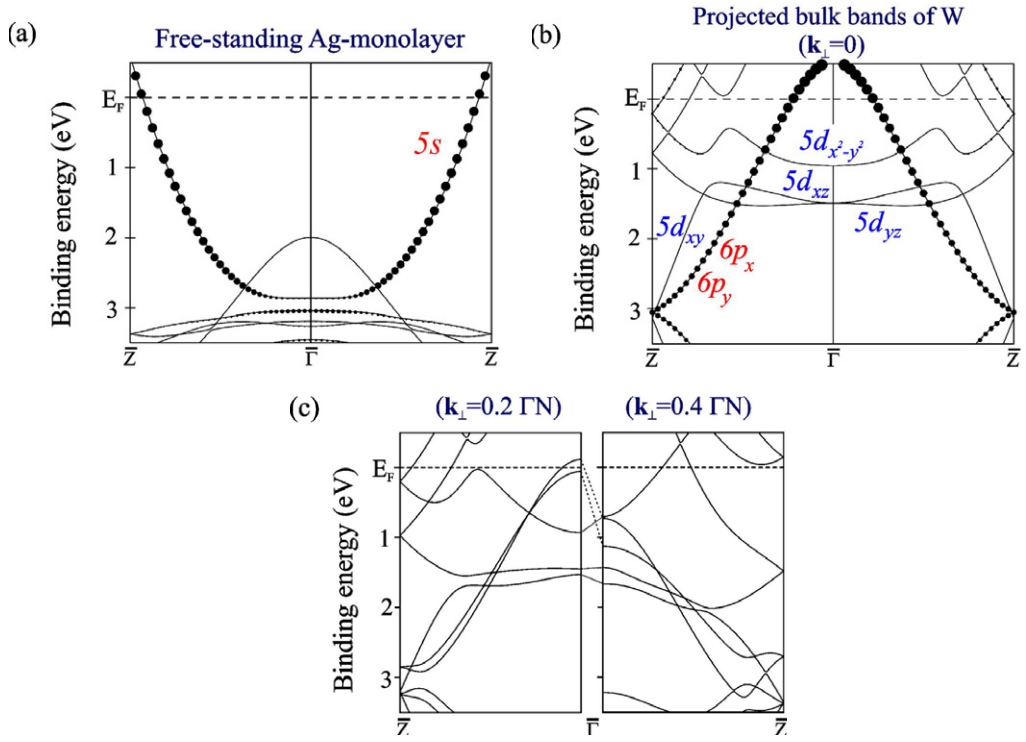

Figure 6. Electronic bands for $\mathbf{k}_{||}$ along the $\overline{\Gamma}$–$\overline{\mathrm{H}}$ ($\overline{\mathrm{Z}}$)-direction for a free-standing Ag monolayer (a), and the bulk W crystal taking $\mathbf{k}_{\perp} = 0$ (b) and $\mathbf{k}_{\perp}$ equal to 20 or 40% of the Γ–N distance. Ag 5s-derived states (a) and W 6p-derived states (b) are denoted by lines through solid dots of diameter proportional to the contribution of the respective states.

to the mirror plane (yz), they do not interact with electron states of the Ag 5s-derived band that are *even* with respect to this mirror plane. All other Ag-derived d bands lie at higher BE.

It should be noted that characterization of the band states in terms of the atomic orbitals means that the respective basis function produces the largest contribution to the Bloch function for the considered $\overline{\Gamma}$–$\overline{\mathrm{H}}$-direction in the surface BZ. Exact symmetries denoted in figure 6 could be assigned to the electronic states only at some high-symmetry $\mathbf{k}$ points (e.g. $\overline{\Gamma}$ point). Then, the spin–orbit coupling leads to additional mixing of partial waves.

Nevertheless, this symmetry characterization is very useful for analyzing the parity of the electron states that is retained within the energy band for all $\mathbf{k}$ points along the considered direction in the surface BZ. We consider now the energy band structure of tungsten. Projecting the bands on the (110)-plane, we take into account only translations parallel to the surface and fix the value of $\mathbf{k}_{\perp}$. Since the component $\mathbf{k}_{\perp}$ is not well defined in ARPES, we have performed calculations for several different $\mathbf{k}_{\perp}$ values. The results of these calculations are presented in figure 6(b) and (c). For $\mathbf{k}_{\perp} = 0$ one sees at the $\overline{\Gamma}$ point pure W 5d states split by the spin–orbit interaction into a $d_{x^2-y^2}$-derived state and a twofold degenerated (d_{xz}, d_{yz})-derived state. With respect to the (yz)-mirror plane only the d_{xz}-derived state is odd. For other $\mathbf{k}$ points of the $\overline{\Gamma}$–$\overline{\mathrm{H}}$-direction the degeneracy of these energy bands is lifted. The odd d_{xz}-derived band hybridize with the d_{xy}-derived band of the same parity (see the band splitting at 1 eV BE). Another band splitting visible just below the Fermi level (crossover of

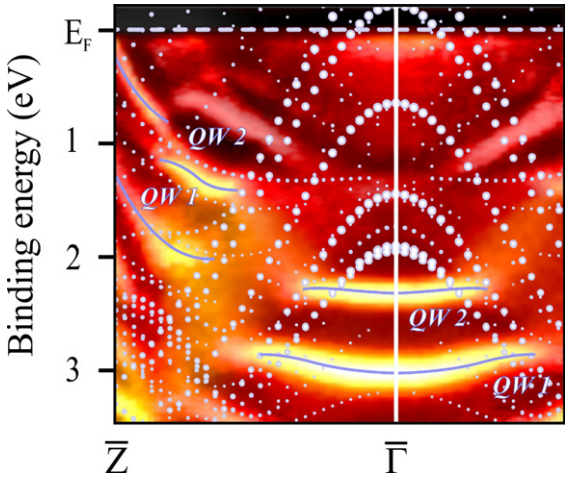

Figure 7. Superposition of experimentally obtained band map for ∼1.5 ML Ag/W(110) with projected W $6p_y$-derived bands to the W(110)-plane for $\mathbf{k}_{||}$ along $\overline{\Gamma} - \overline{\mathrm{H}}$ ($\overline{\mathrm{Z}}$) and $\mathbf{k}_{\perp}$ changing from 0 to the full distance between Γ and N points. Diameter of solid dots is proportional to the $6p_y$ contributions. Solid lines denote guides to the eye for dispersion of the *QW 1* and *QW 2* subbands.

the d_{xy}- and $d_{x^2-y^2}$-derived bands) is caused by spin–orbit coupling. The occupied W $d_{3z^2-r^2}$-derived states lie outside of the energy region of interest (at 5 eV BE). The parabola-like band denoted in figure 6(b) by solid dots is derived from W 6p states and is two-fold degenerate (p_x and p_y states). The band degeneracy is lifted for $\mathbf{k}_{\perp}$ values different from zero (see figure 6(c)) leading to the appearance of two bands that are odd (p_x) and even (p_y) relative to the mirror plane, respectively (note that p_y states are oriented perpendicular to the W(110) surface). Due to their dispersion in the $\mathbf{k}_{\perp}$ direction, these W p bands are shifted to higher BE when going from $\mathbf{k}_{\perp} = 0$ to larger values of $\mathbf{k}_{\perp}$. The W d bands are less sensitive to the $\mathbf{k}_{\perp}$ variations. Nevertheless, for $\mathbf{k}_{\perp} > 0.4\Gamma N$ the energy gap around the $\overline{\Gamma}$ point begins to close. A comparison of the calculated bands with the experimental ARPES data measured for the clean W(110)-surface (see figure 2, top panel) indicates that the PE experiment obviously probes electron states with values of $\mathbf{k}_{\perp}$ close to the BZ plane crossing the Γ point.

Now, we place the Ag monolayer on the W(110)-surface. Thereby a significant charge transfer due to contact potential is not expected, since the workfunctions of the two metals are of similar magnitude. The surface potential barrier at the Ag monolayer on the side adjacent to the W surface is strongly reduced allowing the Ag–W interaction. Certainly, Ag 4d electrons could create bonding states with 5d electrons of the W atoms in the topmost layer. These states are expected at BE of 3 eV and higher. In contrast to the spatially strongly localized Ag 4d states, Ag 5s-derived waves are extended enough to overlap W 5d states even in the second and third atomic layers. This interaction should affect the parabola-like shape of the Ag 5s-derived band. In the energy region of interest (about 2–2.5 eV BE) one can observe two types of W bands that may cross the Ag 5s-derived band, namely, the W $5d_{xy}$- and 6p-derived bands. The W d_{xy} band is odd with respect to the mirror plane-(yz). Therefore, its interaction with the *even* parity Ag 5s-originating band is symmetry forbidden. The same is valid for the W p_x-derived band. Thus, from symmetry requirements the p_y-derived energy band of even parity is the only band that is allowed to hybridize with the Ag 5s-derived band. Obviously, this hybridization is allowed for

all possible values of $\mathbf{k}_\perp$ because of a breakdown of the periodicity of the crystal at the surface along the normal direction. In figure 7, we combined the experimentally obtained band map for ∼1.5 ML Ag deposited on the W(110) with projected W p_y-derived states. For a pictorial view, we enhanced the intensity contrast of the experimentally observed bands. The projected W p_y-derived states form a broad bunch of energy bands crossing in the $E(\mathbf{k}_{||})$ diagram the Ag 5s-derived parabolic band. Interaction between overlayer and substrate states leads to a lifting of energy degeneracy of symmetric and antisymmetric linear combinations and, thus, to the formation of the broad energy gap reflected in the PE data.

Note also that another significant deviation from free-electron-like behaviour for the *QW 2* band is seen close to the $\overline{\mathrm{Z}}$ point within BE range of 0.6–1.3 eV, exactly at the crossover point of the *QW 2* band with the even W $5d_{yz}$-derived band. The W $5d_{x^2-y^2}$-originating band which is also even with respect to the (yz)-mirror plane lies mainly between 1 eV BE and the Fermi level (its tracks can be seen in figure 3 or 7). This band does not cross the existing QW bands.

5. Summary

We have observed an energy-gap formation for Ag-derived QW states around **k** points, where the two-dimensional Ag bands cross the projected bulk bands of the W substrate. This phenomenon is properly reproduced by the LKKR calculation of the ARPES spectra and is caused by hybridization of the Ag 5s-derived QW subband with W 6p-originating states characterized by *even* parity with respect to reflection at the emission plane. On the basis of our results, we conclude that generally observation of an energy-bandgap in the distribution of QW states may be used to probe the parity of extended bands of the substrate. We believe that this approach can be applied successfully for detecting the parity of wave functions of electronic states in strongly correlated electron systems like heavy fermion materials. Even in the case of the quasi-localized 4f states strong interactions with free-electron-like bands have been observed in ARPES spectra [2, 16, 17] that lead to gap formation, very similar to the phenomena reported in the present work.

The symmetry properties of QW states in simple metals, such as Au, Ag, Mg, Al, etc, are well understood. Therefore, from the possible formation of energy gaps in QW bands direct conclusions may be drawn about the related properties of substrate bands in strongly correlated systems that are difficult to handle within an *ab initio* approach due to many body interactions.

Acknowledgments

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References

[1] Borisenko S V *et al* 2006 Parity of the pairing bosons in a high-temperature Pb-$Bi_2Sr_2CaCu_2O_8$ bilayer superconductor by angle-resolved photoemission spectroscopy *Phys. Rev. Lett.* **96** 067001

[2] Danzenbächer S *et al* 2007 Momentum dependence of 4f hybridization in heavy-fermion compounds: angle-resolved photoemission study of $YbIr_2Si_2$ and $YbRh_2Si_2$ *Phys. Rev.* B **75** 045109

[3] Vyalikh D V *et al* 2008 Photoemission insight into heavy-fermion behavior in $YbRh_2Si_2$ *Phys. Rev. Lett.* **100** 056402

[4] Chiang T C 2000 Photoemission studies of quantum well states in thin films *Surf. Sci. Rep.* **39** 181–235
[5] Aballe L, Rogero C, Kratzer P, Gokhale S and Horn K 2001 Probing interface electronic structure with overlayer quantum-well resonances: Al/Si(111) *Phys. Rev. Lett.* **87** 156801
[6] Tang S J, Basile L, Miller T and Chiang T C 2004 Breakup of quasiparticles in thin-film quantum wells *Phys. Rev. Lett.* **93** 216804
[7] Rotenberg E, Wu Y Z, An J M, van Hove M A, Canning A, Wang L W and Qiu Z Q 2006 Non-free-electron momentum- and thickness-dependent evolution of quantum well states in the Cu/Co/Cu(001) system *Phys. Rev.* B **73** 075426
[8] Tang S J, Miller T and Chiang T C 2006 Modification of surface states in ultrathin films via hybridization with the substrate: a study of Ag on Ge *Phys. Rev. Lett.* **96** 036802
[9] Varykhalov A, Shikin A M, Gudat W, Moras P, Grazioli C, Carbone C and Rader O 2005 Probing the ground state electronic structure of a correlated electron system by quantum well states: Ag/Ni(111) *Phys. Rev. Lett.* **95** 247601
[10] Shikin A M, Vyalikh D V, Dedkov Yu S, Prudnikova G V, Adamchuk V K, Weschke| E and Kaindl G 2000 Extended energy range of Ag quantum-well states in Ag(111)/Au(111)/W(110) *Phys. Rev.* B **62** R2303–6
[11] Vyalikh D V, Weschke E, Dedkov Yu S, Kaindl G, Shikin A M and Adamchuk V K 2003 Quantum-well states in bilayers of Ag and Au on W(110) *Surf. Sci. Lett.* **540** L638–42
[12] Deisl C, Bertel E, Burgener M, Meister G and Goldmann A 2005 Epitaxial growth of Ag on W(110) *Phys. Rev.* B **72** 155433
[13] Nemoshkalenko V V, Krasovskii A E, Antonov V N, Antonov Vl N, Fleck U, Wonn H and Ziesche P 1983 The relativistic linear muffin-tin orbital method application to Au *Phys. Status Solidi* B **120** 283–96
[14] Andersen O K 1975 Linear methods in band theory *Phys. Rev.* B **12** 3060–83
[15] Halilov S V, Tamura E, Meinert D, Gollisch H and Feder R 1993 Relativistic Green function theory of layer densities of states and photoemission from magnetic compounds *J. Phys.: Condens. Matter* **5** 3859–70
[16] Danzenbächer S *et al* 2006 Energy dispersion of 4f-derived emissions in photoelectron spectra of the heavy-fermion compound $YbIr_2Si_2$ *Phys. Rev. Lett.* **96** 106402
[17] Vyalikh D V, Kucherenko Yu, Danzenbächer S, Dedkov Yu S, Laubschat C and Molodtsov S L 2006 Wave-vector conservation upon hybridization of 4f and valence-band states observed in photoemission spectra of a Ce monolayer on W(110) *Phys. Rev. Lett.* **96** 026404