**Abstract.** Here we present applications of the periodic Anderson model (PAM) to consideration of wave vector ($k$)- and spin-dependent hybridization effects in Ce metal. It was shown that $k$-dependent splitting of the 4$f$ ionization peak of Ce/W(110) are correctly described in the framework of the PAM (Coulomb repulsion between two $f$ electrons localized on the same lattice site $U_{ff} \to \infty$). Our results show that the wave vector is conserved upon hybridization. In case of the magnetically ordered Ce monolayer, spin- and angle-resolved resonant photoemission spectra reveal spin-dependent changes of the Fermi-level peak intensities (which reflect the hybridization strength). That indicate a spin-dependence of 4$f$ hybridization and, thus, of 4$f$ occupancy and local moment. The phenomenon was also described in the framework of PAM by 4$f$ electron hopping into the exchange split Fe 3$d$ derived bands that form a spin-gap at the Fermi energy around the $\Gamma$ point of the surface Brillouin zone.

The interaction of localized 4$f$ states with itinerant conduction-band states leads to a series of correlation phenomena that have attracted considerable interest in the last few decades. Apart from spin-polarization effects that cause magnetic coupling via the RKKY interaction, hybridization may lead to noninteger $f$ occupations, to heavy fermion behaviour, or even to a breakdown of Fermi-liquid properties [1]. A typical and well studied system is Ce metal where hybridization of the trivalent 4$f^1(5d6s)^3$ with the tetravalent 4$f^0(5d6s)^4$ and divalent 4$f^2(5d6s)^2$ configurations is responsible for the isostructural $\alpha-\gamma$ phase transition related to a volume collapse of 15% and a quenching of the magnetic moment at low temperatures [2]. The Gunnarsson-Schönhammer approach [3] to the single-impurity Anderson model (SIAM) [4] allows one to relate electron spectroscopic data to results of low-energy experiments like specific heat, conductivity, and magnetization measurements and was successfully applied to many rare-earth systems [5]. A natural weakness of SIAM is, however, that it ignores completely the effects of translation symmetry of structurally ordered solids. Consideration of the latter leads to the periodic Anderson model (PAM), for which, however, realistic theoretical approaches are still not available.

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In the present work we apply PAM for the description of hybridization effects in Ce monolayer (ML). Our results show that for the Ce/W(110) the wave vector \( \mathbf{k} \) is conserved upon hybridization and \( \mathbf{k} \)-dependent splitting of the \( 4f \) ionization peak is correctly described in the framework of the PAM. In case of the magnetically ordered Ce monolayer, spin-resolved photoemission (PE) spectroscopy reveals spin-dependent changes of the Fermi-level peak intensities (which reflect the hybridization strength). That indicate a spin-dependence of \( 4f \) hybridization and, thus, of \( 4f \) occupancy and local moment. This phenomenon was correctly described in the framework of PAM by \( 4f \) electron hopping into the exchange split Fe \( 3d \) derived bands.

Spin- and angle-resolved resonant PE experiments at the Ce \( 4d \rightarrow 4f \) absorption threshold were performed using a hemispherical PHOIBOS 150 electron-energy analyzer (SPECS) equipped with a 25 kV mini-Mott spin detector and synchrotron radiation from beamline U125/1-PGM of BESSY (Berlin). The energy and angle resolutions were set to 100 meV and 1\(^\circ\), respectively. The light incidence angle was 30\(^\circ\) with respect to the sample surface. Spin-resolved measurements were performed in normal emission geometry in magnetic remanence after having applied a magnetic field pulse of about 500 Oe along the in-plane \(<1-10>\) easy axis (perpendicular to electric field vector of the light) of the Fe(110) film. The experimental setup asymmetry was accounted for in the standard way by measuring spin-resolved spectra for two opposite directions of applied magnetic field [6,7]. The base pressure in the experimental chamber was in the upper 10\(^{-11}\) mbar range rising shortly to the upper 10\(^{-10}\) mbar range during evaporation and annealing. Prior to the deposition of Fe or/and Ce, the W(110) substrate was carefully cleaned by repeated cycles of heating up to 1300\(^\circ\)C in oxygen atmosphere for 15 min each (with a partial pressure of 5×10\(^{-8}\) mbar) and subsequent flashing at 2300\(^\circ\)C. A structurally ordered monolayer of Ce metal was grown on a W(110) substrate kept at room temperature. A Fe(110) substrate was prepared by thermal deposition of Fe films with a thickness of 50 Å on W(110) and subsequent annealing at 450 K. Low-energy electron diffraction (LEED) yielded sharp...
patterns with two-fold symmetry as expected for a structurally ordered bcc Fe(110) surface. Further deposition of 0.5 ML (close-packed atomic arrangement) of Ce metal at 300 K led to a sharp overstructure in the LEED pattern.

The left panel in Fig. 1 shows a set of angle-resolved PE spectra recorded along the $\overline{K} - \Gamma$ direction of the surface Brillouin zone for the hexagonal $\alpha$-Ce monolayer. One can see that the peak at the Fermi level ($E_F$) indicating large hybridization of the system, remains practically unchanged in both intensity and line shape. However, the same is not true for the ionization peak. When going away from normal emission, it splits in, at least, two components. This energy splitting is maximal for polar emission angles between 2° and 3°. For polar angles larger than 5° this splitting disappears and the shape of the PE spectra shows no significant differences to the one of normal emission.

Electronic and magnetic structures of the Ce/Fe(110) system were probed by spin-resolved resonant PE at the Ce $4d \rightarrow 4f$ absorption edge [Fig. 2(a)]. In order to extract the Ce $4f$ contribution from the observed total-intensity (open/filled circles) as well as majority- (open triangles) and minority-spin (filled triangles) PE spectra, each time the corresponding off-resonance PE spectrum was subtracted from the on-resonance one. The resulted PE spectra together with spin polarization of Ce $4f$ photoelectrons are shown in the upper part of Fig. 2(b) (marked as "EXP."). The total-intensity Ce $4f$ PE spectrum shows a well-known two-peak structure, with a main maximum near 2 eV BE (ionization peak) and a hybridization peak near the Fermi energy. The main observation is that the intensity of hybridization peak is determined predominantly by the minority-spin contribution, whereas for the majority-spin spectrum only a weak shoulder can be distinguished at this binding energy (BE). This fact indicates the effect of spin-dependent 4f hybridization in magnetically ordered Ce layer.

In order to describe the angle- and spin-resolved PE spectra, we used a simplified version of periodic Anderson model [8,9]. In this approach the double occupation of the $4f$ states is ignored and momentum as well as spin conservation upon hybridization is assumed (for details, see [10-12]). For the hybridization matrix element $V_{k}\sigma(E)$ between two electron subsystems (VB and $4f$ states) we use the calculated respective $f$-projected local expansion coefficients $c_{f}(E,k)$ of the Bloch functions around the rare-earth sites: $V_{k}\sigma(E) = \Delta c_{f}(E,k)$, where $\Delta$ is an adjustable hybridization parameter. Expansion coefficients $c_{f}(E,k)$ that characterize the local $f$ character of VB states were taken from the results of band-structure calculations for the La/W(110) and La/Fe(110) system, in order to exclude the contribution of localized Ce $4f$ orbitals.
The results of the calculations for the Ce/W(110) in the Γ-K direction are shown in the inset of right panel in Fig. 1. The energy position of the unhybridized 4f level in Ce metal is about 1.5 eV [13]. Therefore, assuming the 4f states to create a dispersionless band at this energy, this f band should cross the parabolic VB close to a k point corresponding to 3° (Fig. 1). In the region of this point hybridization effects between 4f and VB states are expected.

The calculated PE spectra change their shape with an increase of the emission angle (Fig. 1, right panel). The ionization peak is split into two maxima that diverge from each other by up to about 1 eV. This behavior is in excellent agreement with that observed in the experimental PE spectra. Thus, the splitting of the peak at 2 eV BE in the angle-resolved spectra of the Ce monolayer on the W(110) may be ascribed to the interaction of the 4f states with the parabolic VB that leads to the typical picture of two hybridized energy bands.

In case of the Ce/Fe(110) system, where spin-resolved data were obtained in normal emission geometry we have to consider the VB states at the Γ point of the surface Brillouin zone. The calculated |c|^2 values at this point are given in the bottom part of Fig. 2 (a). As can be seen, the theoretical energy distributions of the VB f states are quite different for the majority- and minority-spin electrons. These VB states of f symmetry in the La atomic sphere are formed by combination of tails of wave functions of the neighboring atoms (mainly Fe 3d) and reflect (to some extent) their energy and spin distribution. The calculated VB f character causes strong differences in the hybridization matrix elements for majority- and minority-spin states resulting in different shapes of the 4f PE spectra for two spin directions.

The calculated spin-resolved Ce 4f PE data presented in the lower part of Fig. 2(b) (marked as "CALC.") agree well with the experimental spectra [Fig. 2(b), "EXP."] and reflect all features observed there. The minority-spin spectrum has much higher intensity of the hybridization peak near the Fermi energy due to high density of the minority-spin VB states in this range of BEs. A shoulder near 1 eV BE is due to the hybridization effects with the peaks in the VB at 0.9 and 1.3 eV. In the calculated majority-spin spectrum no hybridization peak is observed, because of negligibly small density of VB states for this spin direction at the Fermi level. On the other hand, the ionization peak is split in three features (maxima at 0.9 eV, 2.1 eV and shoulder at 3 eV) as a result of hybridization coupling with the VB states (peak at 1.4 eV and VB states between 2 eV and 3 eV). The calculated spin polarization describes qualitatively the energy dependence of the measured polarization. Especially, there is a very good agreement for the points where the spin polarization changes the sign.

In conclusion, angle- and spin-resolved photoelectron spectroscopy was applied for studies of hybridization effects in Ce monolayer. Variation of Ce 4f spectral weights with change of wave vector or spin is explained within the periodic Anderson model by k- and spin-dependent 4f/hybridization.

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