Universität Münster

Aktuelle Fragen der Nanophysik

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ARPES studies of Hf(0001) monocrystal: experiment and theory

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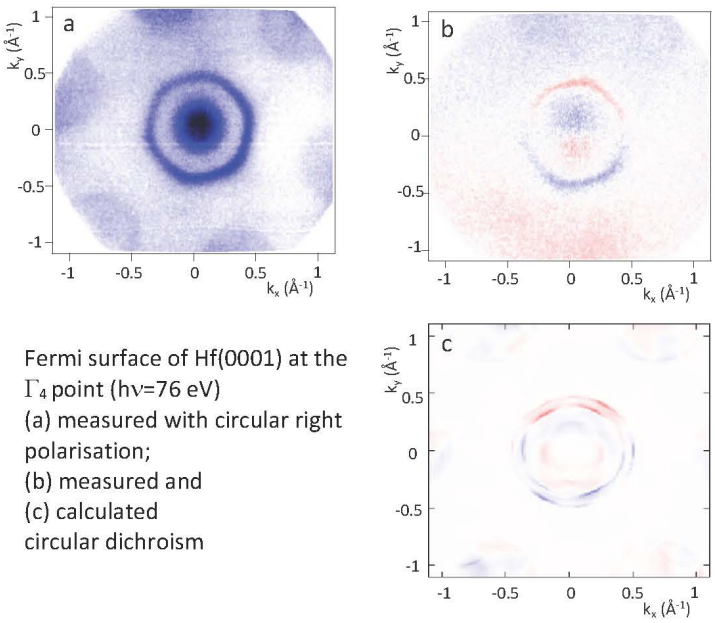
We present first ARPES studies of the electronic structure of the Hf(0001) surface. High-Z materials have attracted much interest, because the strong spin-orbit coupling in combination with the broken inversion symmetry and an important effective electric field at the surface results in a spin-momentum locking [1-3]. Spin-polarized electrons at the surface are of interest in physics and novel applications in electronics and data processing.

Surprisingly, ARPES studies of Hf crystal surfaces are entirely missing in literature. The main effort is concentrated to hafnium-based oxides that replaced, from 2007, the silicon oxide as a gate insulator in field-effect transistors because of their high dielectric constant.

As this is the case for tungsten, the hafnium surface is very sensitive to oxidation. In the cleaning procedure we finely tuned the annealing temperature yielding a high-quality unreconstructed surface. Our ground state as well as one-step calculations are in a very good agreement with measured ARPES spectra. Thanks to ab-initio calculations performed within the SPR-KKR package, we recognized some additional states that can be attributed to oxygen and carbon contaminations of this highly reactive surface.

4f core-level spectra reveal that the surface component at the Hf(0001) surface is situated on the higher binding energy side of the bulk peak, on the contrary to all W crystallographic faces [4], [5].

[1] Varykhalov A. Phys.Rev.Lett. 108, 066804 (2012)
[2] Elmers H. J. et al., Phys.Rev.Res. **2**, 013296 (2020)
[3] Holtmann M et al., Phys.Rev **B 105**, L241412 (2022)
[4] Wertheim G. K. et al.,, Phy.Rev. B 30, 4343 (1984)
[5] Riffe D. M. et al., Phys.Rev.Lett. 63, 1976 (1989)



Fermi surface of Hf(0001) at the Γ_4 point (hν=76 eV)
(a) measured with circular right polarisation;
(b) measured and
(c) calculated
circular dichroism