Ultramicroscopy ■ (■■■■) ■■■–■■■

Contents lists available at ScienceDirect

Ultramicroscopy

journal homepage: www.elsevier.com/locate/ultramic

Spin resolved bandstructure imaging with a high resolution momentum microscope

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ARTICLE INFO

Article history:
Received 3 November 2014
Accepted 22 March 2015

Keywords:
Photoemission
Momentum microscopy
Electronic structure
Spin-orbit coupling
Surface state
Electron spin polarization

ABSTRACT

We present a spin resolving "momentum microscope" for the high resolution imaging of the momentum distribution of photoelectrons. Measurements of the band structure of a Au(111) single crystal surface demonstrate an energy resolution of $\Delta E = 12$ meV and a momentum resolution of $\Delta k_{\parallel} = 0.0049$ Å^{-1}, measured at the line-width of the spin–orbit split Shockley surface state. The relative accuracy of the $k_{\parallel}$ measurement in the order of 10^{-4} Å^{-1} reveals a deviation from the ideal two-dimensional free electron gas model of the Shockley surface state, manifested in a threefold radial symmetry. Spin resolution in the full momentum image is obtained by an imaging spin-filter based on low-energy electron diffraction at a Au passivated Ir(100) single crystal. Using working points at 10.5 eV and 11.5 eV scattering energy with a completely reversed asymmetry of $\pm 60\%$ we demonstrate the efficient mapping of the spin texture of the Au(111) surface state.

1. Introduction

Photoelectron spectroscopy has evolved in the past decades as a powerful tool to understand the electronic properties of solid state systems [1]. Specifically, angle-resolved photoelectron spectroscopy (ARPES) aims at the measurement of the valence electronic structure and band-dispersion near the Fermi energy. Experimental work is abundant and covers almost all areas of modern solid-state and surface physics, like strongly correlated electron systems, high temperature superconductivity, and topological insulators [2–7]. While the spin of the electron is decisive in all of these subjects and spin resolved studies regularly provide important new insights into the underlying physics, the spin of the electron is still only poorly accessible. The reason is the inherently low efficiency of electron spin detectors, as the measurement of the spin of a free electron in an "ideal" Stern–Gerlach type filter is not allowed by quantum mechanics.

A primary example that documents the progress in spin- and angle-resolved photoemission, since the pioneering experiments [8–10], is the emission of polarized electrons from a nonmagnetic surface. One such system that additionally requires high energy and angular resolution is the Rashba splitting of the Shockley surface state of Au(111) [11–13]. Beside being a frequent test case for high resolution ARPES, the spin texture of the surface state consists of two concentric rings with a high degree of spin polarization [14]. Since the first spin resolved measurements [15,16], it became widely used as a reference in spin resolved ARPES, and recently, for understanding peculiar symmetry induced relationships between ground-state- and photoelectron-spin [17–20]. Still, improved experimental and theoretical work reveals limits of the widely accepted picture of the idealized two-dimensional electron gas and the Rashba model [21,22].

On the experimental side, modern hemispherical electron energy analyzers employ a two-dimensional detection scheme to meet the requirements of high resolution spectroscopy. An imaging detector, placed in the open exit plane of the analyzer, measures the emission angle and the energy, simultaneously. Due to the α^2 aberration term inherent to this type of analyzer [23], the ultimate resolution can only be achieved by the restriction to a small volume in phase space. By contrast, most spin detectors used today can only measure one energy- and angular channel at a time [24]. Consequently, a spin-resolved photoemission experiment requires a significant trade-off in resolution. A few recent improvements try to increase the efficiency of the single channel detection, i.e. by exploiting exchange scattering, such that angle resolved experiments in principle became feasible [25,26]. Only recently, two-dimensional spin detection became available for hemispherical analyzers, based on the image conserving reflection of electrons at a crystal surface, resulting in a drastic reduction of measurement time [27].

A different approach for the simultaneous measurement of a two-dimensional photoelectron distribution was introduced by Kotsugi et al. using a photoelectron emission microscope (PEEM)

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http://dx.doi.org/10.1016/j.ultramic.2015.03.020

[28]. In contrast to a conventional ARPES experiment, all electrons that are emitted from the sample into the complete half space are collected by the accelerating electric field between the sample and the microscope objective lens. In this case, the two image coordinates on the detector do not correspond to emission angles, but to the more meaningful transverse momentum, $k_{\parallel}$, of the emitted electron. In this early work, the energy of the photoelectron was fixed to the Fermi edge, limiting the practical use. More recently, a more versatile proof-of-principle of such "momentum microscope" was introduced [29]. This instrument combined a typical PEEM column, as was already used in Ref. [28], with an hemispherical energy analyzer that compensates the α^2 aberration, enabling the fast acquisition of the three-dimensional (k_x, k_y, E) band dispersion. In particular, the data beyond high-symmetry directions provides valuable input for quantitative theoretical models. For instance, the comprehensive data sets allow us to analyze the effect of band renormalization in photoemission theory [30]. The fixed photoemission geometry gives further direct access to symmetry dependent effects and dichroism [31]. The combination of such a photoelectron microscope with an imaging spin filter already showed that several thousand spin-resolved points can be recorded in an energy filtered microscope image [32,33], making this measurement scheme a promising choice for high-resolution photoemission experiments.

In this paper, we present the first measurements conducted with a new spin-resolving momentum microscope, designed to combine high-resolution momentum resolved bandstructure imaging, with the extremely high efficiency of an imaging spin filter. While the previous generation instruments only had limited resolution in the energy- and momentum coordinates, each being at least one order of magnitude behind that of conventional ARPES setups, we demonstrate that this is not a fundamental limitation of the momentum microscopy principle. We underline this with benchmarking measurements of the electronic structure of a Au (111) single crystal, which represents an ideal test case for the performance of the momentum microscope. Using an imaging spin filter based on the specular reflection of low-energy electrons from a Au/Ir(100) target [34], the spin-texture of the Rashba-split surface state is measured. Our results demonstrate that the Au (111) surface state serves as an ideal reference for the resolution and calibration of an imaging spin filter.

2. Description of the momentum microscope

Fig. 1a shows the outline of the momentum microscope system. The most important component is the cathode lens that is formed by the surface of the sample (cathode), kept near ground potential, and the anode at a positive potential. Electrons that are emitted into the complete solid angle above the surface are accelerated towards the anode, and enter the momentum microscope imaging column under a finite angle. This principle allows us to measure emission angles up to $\pm 90°$. The maximum value of the parallel momentum that can be found at a given kinetic energy is limited by the vacuum cut-off, determined by the dispersion relation of the free electron

$$k_{\parallel}^{max} = \beta \cdot \sqrt{E}, \tag{1}$$

where $\beta = \sqrt{2m_e/\hbar^2}$, and E is the kinetic energy of the emitted electron directly above the sample surface.

As the cathode formed by the sample is part of the electron optical system, the mechanical alignment with respect to the anode and the electron optical axis is critical. Therefore, our sample stage is based on a hexapod manipulator that provides alignment in six degrees of freedom. A commercial helium flow cryostat was mounted directly on the hexapod and is moved together with the sample. By measuring the temperature using a silicon diode mounted at the surface of a "dummy" sample, we found a minimum temperature of 18 K.

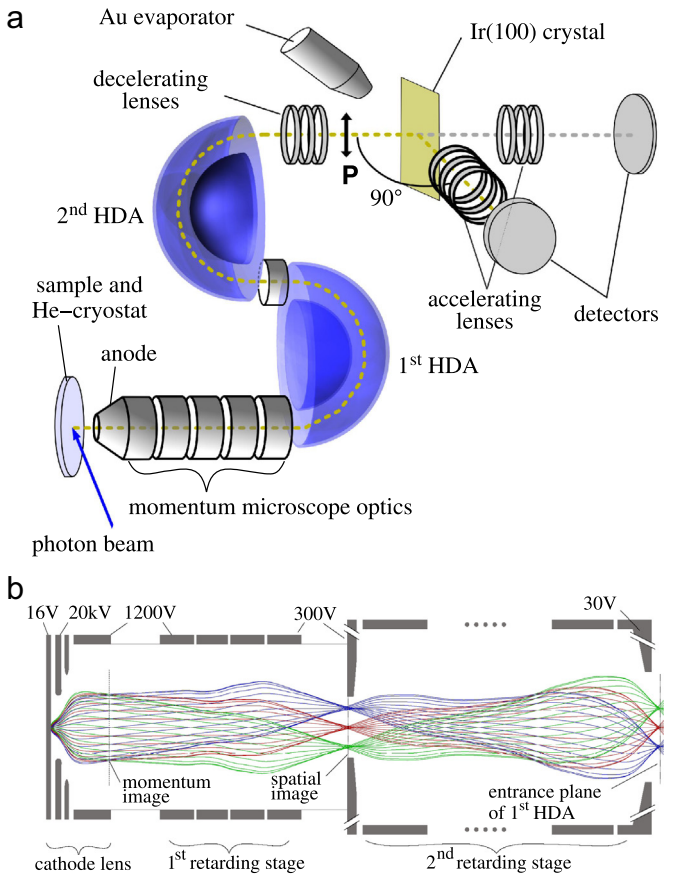

Fig. 1. (a) Outline of the momentum microscope system, consisting of He-cooled sample stage, imaging electron optics, two hemispherical analyzers, and detection branches for spin-integral and spin-filtered imaging. The Ir(100) crystal can be inserted/retracted after the 2nd HDA. (b) Detail of the momentum microscope optics with schematic arrangement of electrodes and trajectories of 16 eV electrons emitted from the sample.

Energy filtering of the photoelectrons is accomplished by a combination of two hemispherical deflection analyzers (HDAs). Each hemisphere has a mean radius of $r_0 = 150$ mm and was modified from a commercially available electron spectrometer (PHOIBOS 150, Specs GmbH). Electrons that pass the entrance plane of the first analyzer are deflected in the spherically symmetric $1/r$ potential, and have the largest energy dispersion after a deflection of 180°. The image obtained in the exit plane of the first HDA is energy dispersed and subject to the α^2 aberration [23]. An effective refocusing of the electron trajectories was described in Ref. [35] by using an electrostatic lens to couple the trajectories to the entrance of the second HDA, such that an effective 360° deflection path is realized. The same principle was also used in previous work [29] and is described in detail in Refs. [36,37]. In short, the solution for a 360° deflection in the spherical $1/r$ potential is a well-known problem in classical mechanics and leads to closed trajectories (Kepler ellipses). By this symmetry, electron trajectories are refocused in the exit plane of the second HDA to the same spatial and angular coordinates as was the starting point in the entrance plane of the first HDA, transmitting the full image information.

Fig. 1b shows the electron optical principle of the momentum microscope imaging column with simulated electron trajectories between the sample and the entrance plane of the first HDA at a

Please cite this article as: C. Tusche, et al., Spin resolved bandstructure imaging with a high resolution momentum microscope, Ultramicroscopy (2015), http://dx.doi.org/10.1016/j.ultramic.2015.03.020