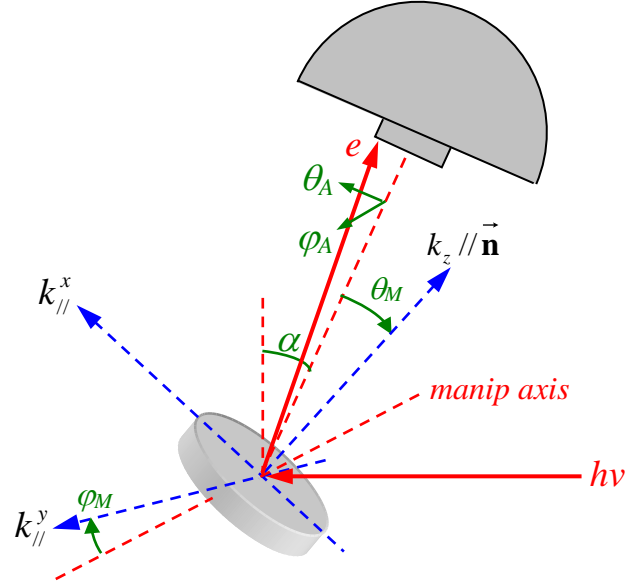


Electron momentum calculations

Geometry of the SX-ARPES experiment at the ADDRESS beamline is shown on the figure. The horizontal incident photon beam and analyser axis form the vertical measurement plane (MP). The analyser axis is inclined by $\alpha = 20^\circ$. The manipulator axis is horizontal and perpendicular to the MP. The parallel momentum $k_{//}^x$ is varied through the *primary* manipulator rotation θ_M , and $k_{//}^y$ through the *tilt* φ_M . The analyser slit can be oriented either in the MP or perpendicular to it, θ_A and φ_A being the angles along the analyzer slit in these two cases. The origin and sign convention for θ_M , φ_M , θ_A and φ_A is indicated on the figure. Note that with this convention the increase of each of these coordinates increases the corresponding $k_{//}$.



The photon momentum is calculated as

$$p_{ph} = \frac{2\pi}{12400} hv$$

Hereinafter the momenta are measured in \AA^{-1} and energies in eV.

With our sign convention, the two parallel momentum components of the *initial (photohole) state* can be found as

$$k_x = 0.5124 \sqrt{hv - e\phi + E_B} \sin(\vartheta_A + \vartheta_M) - 2\pi \cdot hv \cdot \cos(\alpha + \vartheta_M) / 12400$$

$$k_y = 0.5124 \sqrt{hv - e\phi + E_B} \sin(\varphi_A + \varphi_M) \cos(\vartheta_A + \vartheta_M) + 2\pi \cdot hv \cdot \sin(\alpha + \vartheta_M) \sin \varphi_M / 12400$$

where $e\phi > 0$ is the workfunction, $E_B < 0$ binding energy, $\varphi_A = 0$ if the slit is oriented in the MP and $\theta_A = 0$ if perpendicular to it, and ϑ_N is the surface normal angle relative to the analyzer axis (in the shown case $\vartheta_N < 0$). Note that (1) the second term accounts for p_{ph} and does not depend on the θ_A/φ_A angles along the slit; (2) due to rather grazing light incidence in our case, the photon momentum correction to $k_{//}^y$ is small near the normal emission (at $hv = 1000$ eV, $\theta_M = 0$ and $\varphi_M = 10^\circ$, for example, the correction is only $\sim 0.03 \text{ \AA}^{-1}$) but increases at larger θ_M and φ_M .

For the perpendicular momentum,

$$k_z = 0.5124 \sqrt{hv + E_B + V_{000} - 3.81((k_x^f)^2 + (k_y^f)^2)} + 2\pi \cdot hv \cdot \sin(\alpha + \vartheta_M) / 12400,$$

where $V_{000} > 0$ is the inner potential relative to E_F , and $k_x^f = 0.5124 \sqrt{hv - e\phi + E_B} \sin(\vartheta_A + \vartheta_M)$ and $k_y^f = 0.5124 \sqrt{hv - e\phi + E_B} \sin(\varphi_A + \varphi_M) \cos(\vartheta_A + \vartheta_M)$ are the final state (without the p_{ph} -correction) parallel momentum components.