1 Disclamer

Even though this manual pretend to be correct, think twice before doing everything, as temporary changes at the chambers/ instruments might be present at the moment.

This manual has to be considered only as a very basic guide for apes, so do not be offended by the simplicity and poverty of language, either by the numerous grammar/typesetting mistakes (please let the Ape know about them, he will try to correct them).

2 How the analyser works

Everybody knows that the introduction of the surface breaks the translational periodicity of the crystal in the z direction and the wave vector in that direction k_z is thus no longer well-defined. The components of the wave vector parallel to the surface ($k_\parallel$), on the other hand, are still well defined and must be conserved in the photoemission process. They are thus obtained from the photoemission angle with respect to the normal of the sample and the kinetic energy of the photoelectron. In order to map the photoemission intensity on the hemisphere over the sample's surface, it is possible to implement an azimuthal scan (rotating the sample around the surface normal direction) for every polar angle considered. In today's ARPES setups, the electron analyzer often contains a two-dimensional detector that can simultaneously image the energy dispersion of the electrons and the angular dispersion in one direction (see Fig. 1). In this case, it is useful to consider the dispersion along two polar angles (θ and ϕ), along orthogonal directions as presented in Fig. 1(d) (k-warp). In this configuration, the relation between the angles and $\mathbf{k}_\parallel$ is

$$\mathbf{k}_\parallel = (\sin(\phi)\hat{\mathbf{x}} + \cos(\phi)\sin(\theta)\hat{\mathbf{y}}) \cdot \sqrt{\frac{2m_e E_{\text{kin}}}{\hbar^2}}, \tag{1}$$

The SPECS Phoibos 150 spectromiter consists of three main parts (see Fig. 1). A system of cylindrical electrostatic lenses focuses the photoemitted electron beam into an entrance slit that separates the lenses from the hemispherical part. The latter consists of two concentric hemispheres where to different negative potentials are applied that make them work as a passband filter. The potentials are tuned such that only electrons that have an energy between $E_p - \Delta$ and $E_p + \Delta$ can reach a two-dimensional detector as shown in figure Fig.1. E_p is called pass energy and defines the energy resolution of the analyser. In the plain that contains the lenses and the detector (dispersive plane) the energy is so discerned while the advanced system of lenses facilitates the the angular information to be carried to the detector. Only electron emitted in a direction $+\beta$ and $-\beta$ (where β is defined by the voltages on the lenses) in respect to the longitudinal axis of the lenses are able to reach the detector. The lenses are the main core of this system as they not only set a small acceptance angle in the direction parallel to the dispersive plane but also conserve the momentum direction of the photo-electron in a plane that contains the axis of the lenses and orthogonal to the dispersive plane . Further more the lenses reduce by a constant amount the kinetic energy of the incoming electrons in such a way that the electrons with the desired kinetic energy reach the entrance slit with an energy of E_p. The advance of such analyser is that instead of giving as output in single shot a set of intensity profiles versus kinetic energy (EDC- energy distribution curve) at different ϕ angles for a given θ. This property defines the scheme and the geometry of the experiment that is depicted in Fig. 1. A complete map of the Fermi surface can be than obtained by simply rotating the sample in front of the analyser around an axis orthogonal to the dispersive plane and acquiring a spectra for each θ. Each spectra will then be acquired in the form of an image that gives in contrast scale the photoemission intensity versus kinetic anergy for every ϕ angle between $+\beta$ and $-\beta$. This three dimensional dataset

$I(E_{\rm kin}, \theta, \phi)$ obtained by stacking the images will than allow to map the spectral function along different directions in the surface Brillouin zone.

There aresome aberrations to be considered and they are mainly of two types, one in energy, known as astigmatism, and one in the angular dimension. The first one is chronic for hemispherical analysers and leads electrons with same kinetic energy to appear as having different kinetic energies in function of the emission angle. This means, for example, that a constant fermi edge in function of the photoemission angle appears dispersing with angle miming the curvature of the hemispheres. This is known to be easily corrected using a curved entrance slit into the hemisphere. The angular aberration instead brings electrons with different kinetic energies but photoemitted in the same direction to be detected ad different emission angles. Even the latter aberration comes from the spherical geometry of the analyser and can be either corrected tuning the lenses or offline via software. The latter deformation is known either from the specifications of the instrument or from tests that can be run with model systems (e.g. the Au(111) or Cu(111) surface states) and thus the original angular dispersion can be recovered with a warping procedure (anglewarp).

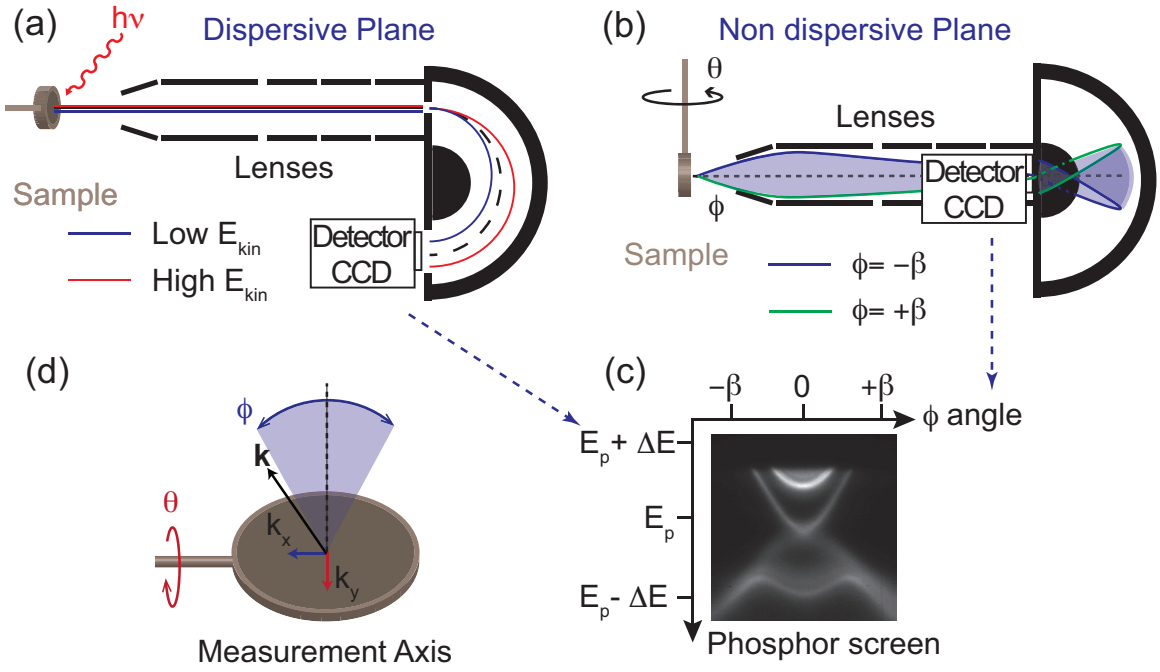

Figure 1: Scheme depicting the hemispherical analyser and the geometry of the ARPES experiment. (a) Cross section and definition of the dispersive plane of the analyser with the orbits of the higher (lower) kinetic energy electrons in red (blue). (b) Cross section of the non dispersive planes of the analyser with the orbits of the electrons emitted at an angle $+\beta$ ($-\beta$) in green (blue). (c) CCD picture of the acquired spectra on the detector. d) Scheme presenting the θ and ϕ angles used to map the photoemission intensity in the experiments performed.

3 How the the beamline works

4 Design of the endstation.

Figs. 2 and 3 show an overview of the new end-station from the top and from the side respectively. The overall system is similar to the previous one: a load lock (LL) is mounted on a preparation chamber (PC1) that is connected via a valve to a main chamber (MC). PC1 is the original one, however a modification of the LL was necessary in order to accommodate a commercial Aarhus STM that will be mounted on the CF150 flange indicated by the green arrow in Fig. 2. Considering the scientific experiments presented in this work, the importance of being able to perform *in situ* STM measurements is clear.

PC1 will be pumped as before by: a cryo-pump, a Ti sublimation pump, an ion-pump, and a magnetic levitating turbo-pump; the rough pumping is shared with the LL via a set of valves. A shortening of the pumping tube was necessary, where the turbo-pump and the ion-pump are placed. This was done to make the pumping more efficient, fit the entire system in the new lower setup and let the human operations on it be more convenient.

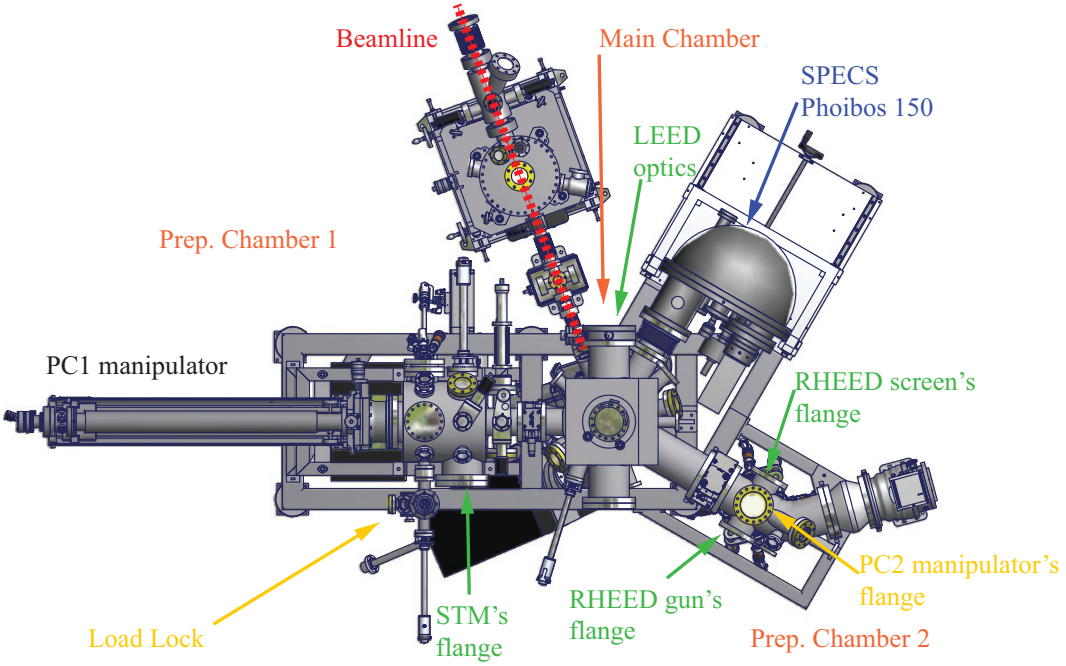

Figure 2: Top view of the new SGM3 end-station with the last mirror of the beamline whose axis is indicated by the red dashed line. Red arrows indicate the main bodies of the end-station, the green ones indicate the measurement instruments, in blue the analyser and in yellow the LL and the PC2 elements are indicated.

The LL has been modified also to be used, when not occupied in the loading of a sample into UHV, as a supplementary pumping system for gas-lines, the rotational feedthrough etc.. This will be pumped by a magnetically levitating turbo-pump. The MC is a μ-metal chamber, smaller than the previous one, thanks to the absence of the old VG Scienta analyser. This chamber can be divided into two levels. At the highest level the transfer of samples from PC1 and LEED measurements are performed. At the lowest level the ARPES data are acquired and transfers to

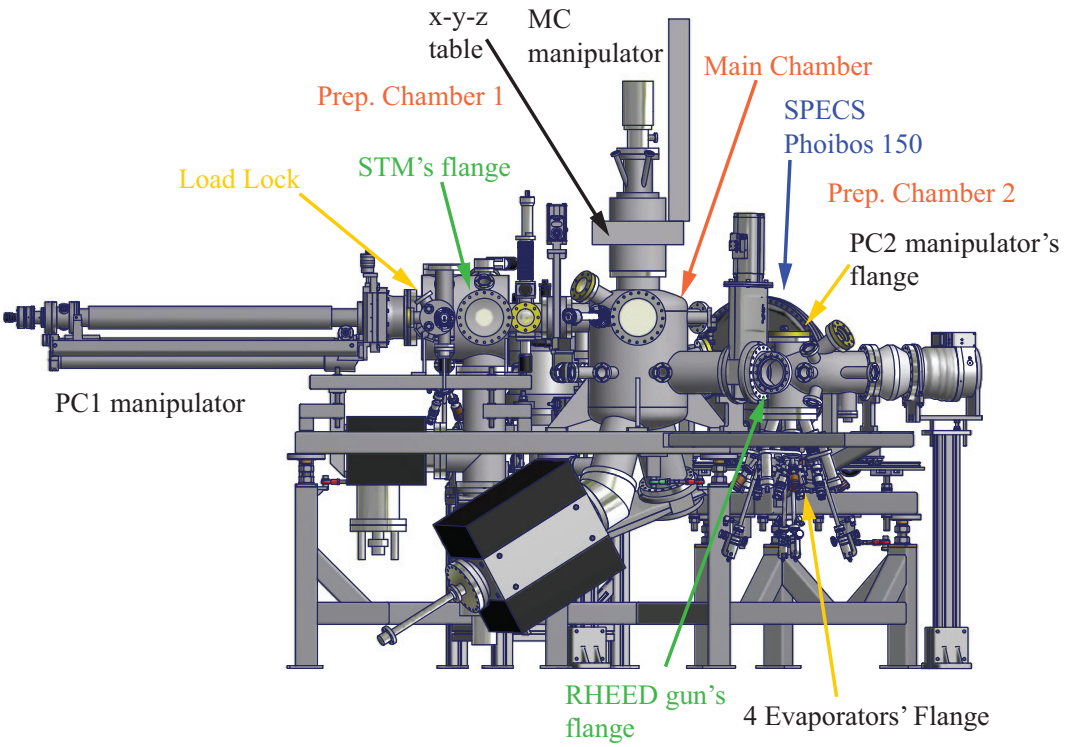

Figure 3: Side view of the new SGM3 end-station from the side opposite to the beamline. Red arrows indicate the main bodies of the end-station, green ones indicate the measurement instruments, in blue the analyser and in yellow the LL and the PC2 elements are indicated.

a second preparation chamber (PC2) are done.

PC2 is a new chamber and it is where the epitaxial growth of crystals can be performed in a controlled way. It is pumped by a magnetically levitating turbo-pump and the rough pump is a scroll pump. PC2 is equipped with:

- a CF150 flange able to host up to 4 retractable evaporators mounted vertically, or 3 evaporators and a sputter gun;
- a manipulator with 2 degrees of freedom, where the sample will be held facing down towards the evaporators;
- a RHEED[1] system that allows the monitoring of the thin film growth;
- a "Tungsten heater"[2], where a sample can be heated to high temperature using e-bombardment, monitoring the temperature with a pyrometer;
- a gas line or a sputtergun;
- a long magnetic transfer arm with a rotating shaft for the transfer to the MC (not shown).

[1] Reflection High Energy Electron Diffraction

[2] This has been inspired by our collaborators in Hamburg and it minimises the degassing during the heating procedure.

The MC remains the core of the end-station and it has been designed to fulfil the following requirements:

- be as small as possible;
- compatibility with both the original and the new manipulators;
- hosting the SPECS Phoibos 150 analyser, the beamline and the LEED optics;
- be magnetically shielded at the ARPES position[3];
- allow the view of the chamber's interior during the transfer of samples;
- flexibility to accommodate an XPS source or eventually evaporators;
- must be easily mountable, in order to facilitate its alignment with the beamline.

Furthermore the LEED optics and the analyser must be oriented so that the transfer from the LEED acquisition position to the ARPES one (and vice versa) is as fast as possible. The LEED optics should also be oriented so that LEED measurements can be performed even while holding the sample on the PC manipulator[4] or rotating azimuthally the sample on the PC socket[5]. A

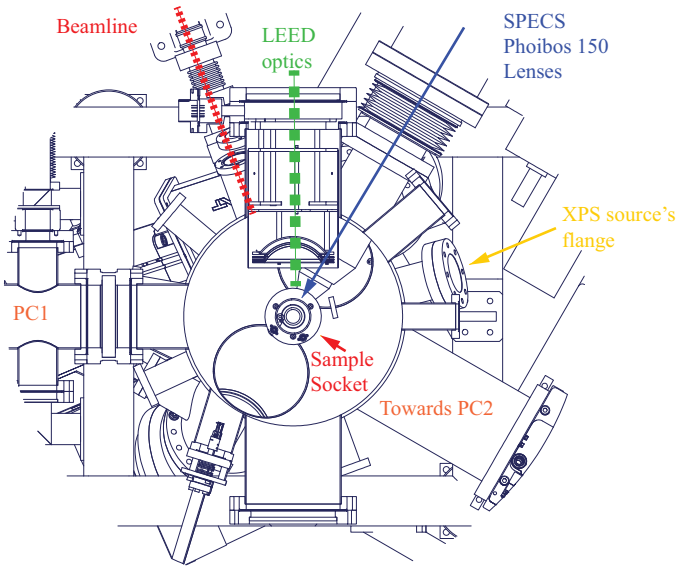

Figure 4: 2D horizontal section of the MC at the LEED optics level. A green dashed line indicates the LEED optics' axis while a solid blue arrow indicates that of the analyser. The top of the socket is also visible at the centre of the chamber.

detail of a 2D horizontal section of the MC is shown in Fig. 4, that should help to clarify the

[3]Even though being μ-metal, this requirement put constraints on the length of the flanges' neck depending on their diameter.

[4]Due to gravity the sample can fall off the PC manipulator. This originates ultimately from the design of the sample holder and socket.

[5]This possibility has been blocked recently as in the past this turned out to be a convoluted procedure for an external user. In order to reach the LEED measurement position, one should rotate both the sample and the manipulator with a very high risk of losing the sample.

fulfilment of these requirements. Thanks to our collaborators' care and patience, all the transfers and movements in vacuum have been checked virtually using CAD software.

When normally operating, the MC is pumped by a Ti sublimation pump, a cryo-pump, an ion-pump and a NEG-pump (Non-Evaporable Getter pump). These are at the bottom of the chamber, looking at the ARPES measurement position from the bottom. However, in the case of the ion-pump, where a magnetic field is present, this has been placed as far away as possible from the analyser and the measurement position. The MC can also be pumped by the turbo-pumps both via PC2 or via PC1. This will become handy in situations where a high pumping speed is desirable, for example during baking or for measurements of the type shown in Fig. **??**.

Last but not least, an important detail has to be considered that is the frame holding in place the end-station. This must allow its fine alignment: the focus of the beamline (the light) and that of the analyser, the centre of rotation of the sample[6] and the surface of the sample must, in fact, coincide.

To accomplish this, the frame is made up of three bodies. A lower body, equipped with wheels and stoppers, is used for the macroscopic movements and the secure placement of the end-station. Another frame (labelled central) is mounted on top of the previous one. This allows the fine movements of the end-station, through acting on bolts and pullers, in all the directions with respect to the light focus (strictly speaking: up, down, left, right and tilt). A smaller frame is finally fixed on top of the central one; this allows the analyser movement with respect to the MC so as to adjust the focus of the lenses. Note that the entire end-station, i.e. LL, PC1, MC, PC2 and analyser moves rigidly together when adjusting the central frame.

The choice of magnetically levitating turbo-pumps and the use of vibrational dampers is justified by the goal of low vibration. This, according to their technical specifications, should allow the operation of the Aarhus STM even without having the chamber on levitating feet. *In extremis*, a system of valves can be closed allowing the turbo-pumps to be shut down, leaving PC1 pumped only by the ion-pump.

The detail that still need to be investigated is the cryostat used for the MC manipulator. This cryostat, being an expander (which is essentially a reciprocating piston), is actually the source of most of the vibrations on the chamber. Until a new, low vibration, closed-cycle He cryostat compatible with UHV becomes available on the market, we will continue to use the original one, taking care to turn it off during the STM measurements.

In order to hold the heavy and long PC1 manipulator mounted horizontally, either a suspended crane or a vertical support from the floor is needed. We have solved this issue similarly to what has been done in the original design, using a system of pulleys and counterweights. This simple idea has been further augmented by the use of a suspended double track that allows us to hold and dismount the PC manipulator easily, without the need for a crane. Using a bifurcation, it also holds the old and the new MC manipulators simultaneously, facilitating their exchange. A crane for additional maintenance will also be present on one of the tracks.

4.1 The 6 axis manipulator

The project of this manipulator has been inspired by the group of Prof. Karsten Horn[7] who we acknowledge also for useful discussions and collaboration.

The manipulator is mounted with its z-drive as the original one on a x-y table that allows μm movements of the manipulator (and therefore of the sample) in the three Cartesian directions. The table is mounted on the same rotatable flange (rotational feedthrough) that is used in the

[6] These are the MC manipulator rotations.

[7] Electronic Structure of Surfaces and Interfaces group, Department of Physical Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.

original setup to perform the polar (θ) rotations during the ARPES scan. The core of the manipulator is the head, where the copper socket holding the sample is mounted on a support (Fig. 5 (a)) that holds also the long rotating shafts implementing the rotations. The particulars of the head's design are presented in Fig. 5 where the sample front (b) and rear (c) side are shown. The head is made of three independently-moving copper bodies that, starting from the

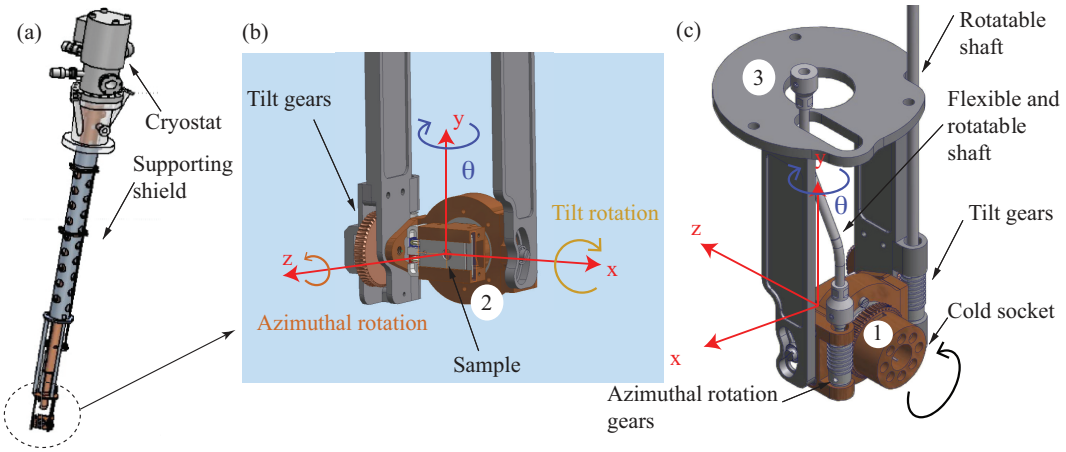

Figure 5: Schematics of the new manipulator (a) with particulars of the new sample socket from the sample front (b) and rear (c) side respectively. The manipulator linear translations are indicated by the red arrows. Orange arrows in (b) and black in (c) indicate the new degrees of freedom which are automatically controlled. The blue arrows in (b) and (c) indicate the θ rotation also available in original manipulator. Numbers inscribed in circles are consistent with the labelling given in the text.

sample holder going towards the manipulator, are:

1. a central cylinder actuating the azimuthal rotations and holding the sample, heating filament and thermocouples;
2. a horseshoe-shaped body that holds the former and actuates the tilt rotation;
3. a C shaped frame holding everything in place.

Two sets of worm gears separately mounted on 1 and 2 provide tilt and azimuthal rotations. The design is intended to be easily maintained and repaired and solid enough to support (and allow) the transfer of the sample many times per day.

Note that 3 is supported by an outer shield on the manipulator, which also holds the rotating shafts, and is therefore at room temperature. Only 1 is connected directly to the cryostat on the top of the manipulator via a flexible copper braid on the back (not shown in Fig. 5). All the thermal insulation between stages 1, 2 and 3 is achieved with a careful choice of materials, knowing that the junction between a metal and a ceramic, or a metal and a plastic material results in a thermally insulating junction.

In particular, where the dimensions allow it, ceramic ball-bearings (in particular ZrO_2) will be used, and where this is not possible, metallic ball-bearings with a PEEK[8] retainer are adopted. Concerning the worm gears, representing a possible heat source, the choice has been to use a metallic worm wheel with a PEEK worm screw. Our collaborators using a similar design were

[8]PolyEther Ether Ketone is a commonly used organic polymer thermoplastic in engineering applications that is practically UHV compatible.

able to reach a lower temperature than the existing manipulator using an open cycle of liquid He and metallic bearings. Note that all these parts, aside from the ceramic bearings, are either easily machinable in the department's workshop or can be quickly purchased for replacements.

The shafts actuating the two additional sample rotations are connected to a rotatable feedthrough on the top of the manipulator. These are moved by two stepper motors controlled by the acquisition software. The issues concerning such a manipulator are the size of the external shield holding the shafts and the head, and the overall weight of the manipulator with cryostat, x-y table and z-drive. The last problem concerns the ability of both the MC and the rotatable flange[9] to bear the weight of the manipulator without deforming[10]. This is solved by the system of pulleys and counter weights that holds the manipulator's weight.

Note that now all the degrees of freedom are remotely controlled (in the previous system only the θ rotations was remotely controlled). This opens new possibilities for ARPES acquisition schemes, e.g. the acquisition of a real azimuthal scan keeping the incident light at constant angle during Fermi surface mapping, and it allows the detection of all the high symmetry directions in a hν-scan without the need to physically remount the sample with a different orientation.

5 Computers' name, tasks and softwares

5.1 Computers

Pepelac (Silver Mac, Dual 1.8 GHz PowerPC G5). Data analysis, Data storage and backups (Marco's office);

st-d01241 (BigMac). Data analysis, Data storage and backups;

Pupken :(black DELL, PC) users computer, back-up of acquisition software, pressure readings in MC and MBE;

nf-a03811 :(black DELL, PC) Data acquisitions with Specs Phoibos 150, Beam-line control, Main chamber movements;

Shirva : (PC) Mass Spectrometer control (no internet connection);

Rigcarn : (PC) Auger Analyser control (no internet connection).

5.2 Main Softwares

5.2.1 Console - ConSys: Angles, Valves, hν, bakeout

The console is installed on Pupken and nf-a03811, and it allows the check/move and control of angles, valves, bakeout and beamline. There are 4 pop-up menus on the top left. The first one should be always blank (the second choice is FEC 04). The second and the third are the important ones. In this manual each time you find e.g. "SRbeamlines ⇒ SGM3 motors: MANANGLE" means "Second pop-up ⇒ third pop-up: blue and green window name".

- beam-line valves and gauges: A2 SGM23 ⇒ A2 SGM23 Vacuum;
- Undulator: A2 Insertion Devices ⇒ A2 WUN 131;

[9] This can hold a maximum of 80 Kg.
[10] Unfortunately μ-metal is softer than stainless steel.