Details of $1\pi$ sr wide acceptance angle electrostatic lens for electron energy and two-dimensional angular distribution analysis combined with real space imaging

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A B S T R A C T
We propose a new $1\pi$ sr Wide Acceptance Angle Electrostatic Lens (WAAEL), which works as a photoemission electron microscope (PEEM), a highly sensitive display-type electron energy and two-dimensional angular distribution analyzer. It can display two-dimensional angular distributions of charged particles within the acceptance angle of $\pm 60^\circ$ that is much larger than the largest acceptance angle range so far and comparable to the display-type spherical mirror analyzer developed by Daimon et al. [1]. It has good focusing capabilities with 5-times magnification and 27(4) $\mu$m lateral-resolution. The relative energy resolution is typically from 2 to $5 \times 10^{-3}$ depending on the diameter of energy aperture and the emission area on the sample.

Although, the lateral resolution of the presented lens is far from those are available nowadays, but this is the first working model that can form images using charged particles collected from $1\pi$ sr wide acceptance angle. The realization of such lens system is one of the first possible steps towards reaching the field of imaging type atomic resolution electron microscopy Feynman et al. [2]. Here some preliminary results are shown.

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1. Introduction

Photoelectron spectroscopy is a powerful technique to study both electronic and atomic structures of solid materials and surfaces [3] and the two-dimensional angle-resolved version of it provides a rich variety of information [4–6]. In the ultraviolet photoelectron spectroscopy (UPS) region the two-dimensional angular distribution of the constant kinetic energy (binding energy) photoelectron reveals the shape of the valence band cross-section and the atomic orbital constituting the valence band [5]. One of the applications of this is the Fermi surface mapping [7] that is especially important because the electronic and chemical characters of materials are determined mostly by the motion of electrons at the Fermi level. Two-dimensional photoelectron angular distribution in the x-ray photoelectron spectroscopy (XPS) region [8] is also powerful in the analysis of three-dimensional atomic structures around specific atoms when photoelectron diffraction (PED) or photoelectron holography (PEH) is applied. Very recently a new method of taking “stereo photograph of atomic arrangements” was invented [9] utilizing the phenomenon of “rotation of forward focusing peaks” [10–12]. The stereoscopic photographs of atomic arrangements can be displayed directly on the screen of a display-type spherical mirror analyzer [1,13,14] without any computer-aided conversion process.

Concentric hemispherical analyzer (CHA) is widely used for angle-resolved photoelectron spectroscopy in virtue of its high energy resolution. Recent development of high performance commercial analyzers and strong synchrotron radiation sources has made it to be able measuring two-dimensional angular distributions easily. In these cases the sample is usually rotated around two axes while the direction of the incident light and detectors are fixed, since the light source and the detector are tending to be large and difficult to rotate around the sample. In photoelectron excitation process the symmetry relation, respected to the electric vector of the linearly polarized light, is important and can be used to distinguish the symmetry of the initial state, especially to determine the atomic orbital constituting the energy band [5]. However, it requires a lot of time to take full-solid-angle angular distribution with CHA because the acceptance angle is narrow, about $7 \times 1$ square degree ($0.001\pi$ sr).
The cylindrical mirror analyzer (CMA) has a wide acceptance angle therefore, it is often used in angular distribution measurements. It collects 42 square degree regions, which corresponds to about 0.23\(\pi\) sr.

A display-type analyzer can measure wide angular distribution of photoelectrons of one particular kinetic energy without changing the angles of incident light and the sample. Eastman et al. [15] developed an ellipsoidal mirror analyzer (DIANA) developed by Daimon [1,13] that displays photoelectrons from \(\pm 43^\circ\) acceptance angle, but is limited by the imperfections of the beam convergence and angular distribution. The display-type spherical mirror analyzer (DIANA) developed by Daimon [1,13] has no angular distortion up to \(2\pi\) sr solid angle and its acceptance angle is limited by the size of MCP to \(\pm 60^\circ\), which corresponds to \(1\pi\) sr. The recent high-energy resolution-type analyzer [14,16,17] has a complicated outer sphere, but when the acceptance angle is limited to \(\pm 20^\circ\) (0.12\(\pi\) sr) a simple outer sphere can be used, which was realized recently by Sakai et al. [18].

In this paper we propose a new wide acceptance angle electrostatic lens (WAAEL) up to \(\pm 60^\circ\) (1\(\pi\) sr), which combines the advantages of display-type analyzers with the capabilities of photoemission electron microscopes using newly developed electron optical elements [19–21], energy apertures [22,23] and some additional components.

2. System configuration and the main properties

Fig. 1 shows a schematic drawing of Wide Acceptance Angle Electrostatic Lens (WAAEL), without deflectors, which was partly described in a previous paper [22,23], and is described in detail here. Some trajectories of the electrons from a point source for three different kinetic energies are shown in Fig. 1. The electron beams with an energy \(E_0\) focus at the focal or with other words aperture plane \(Z=Z_0\), where the acceptance angle \(\alpha\) of \(\pm 60^\circ\) is reduced to \(\pm 12^\circ\), and a five-times magnified image of the sample is created. The electron beams with energies different from \(E_0\) focus at different points, but do not focus at the aperture plane. Hence, energy analysis is realized when we put a small aperture there.

The most important component of WAAEL is an almost ellipsoidal shape mesh [19–21] (Fig. 1) with more than 60\% transmittance where the accurate fabrication determines the focusing spot size of WAAEL [23]. The, WAAEL has a capability of \(1\pi\) sr acceptance angle high sensitive display-type electron energy and two-dimensional angular distribution analyzer similar to DIANA, moreover works as a low-magnification photoemission electron microscope (PEEM).

The biggest advantage of WAAEL over DIANA is that the position of the detector (MCP+screen) is far from the sample. The space around the sample is limited in DIANA because the sample and the detector are close to each other. In WAAEL, the space around the sample is unlimited at right angles to the optical axes (Fig. 1) so even a large wafer can be analyzed.

Another advantage of WAAEL over DIANA is that it does not require a big MCP, because the image or angular distribution size can be controlled by the lenses. The biggest size of available MCP was about 120 mm, which limits the acceptance angle to be less than \(\pm 60^\circ\) in DIANA, because the size of the retardation grids cannot be as small as they must be resistant against high voltages. Even if retardation grids are attached to WAAEL for high-pass filtering, a big MCP is not necessary because the detection angle is more than five times reduced.

A disadvantage of WAAEL over DIANA is that the energy spectrum has a long tail, which is unavoidable in this type of focus–defocus analyzer, as is discussed later in this paper.

In this way, WAAEL can be used in three different modes like energy analyzer, photoemission electron microscope (PEEM) and two-dimensional angular distribution analyzer. In the following, we describe the design and fabrication, as well as the performance as energy analyzer, photoemission electron microscope and angular distribution analyzer together with showing some experimental data.

3. Design and fabrication

The original ray-tracing calculations were made by Matsuda et al. [19-21]. For structural design Solid Edge 3D Cad (Fig. 2) [25] and QCad 2D free [26] software were used, as well as Borland Kylix free software development environment [27] for additional design and calculations.

Furthermore, the effect of the final geometry of the real fabricated parts on the electrostatic field was simulated using SIMION Ion and Electron Optics Simulator (Fig. 3) [28]. The effects of thermal expansion and other mechanical difficulties were also taken into account to achieve higher accuracy.

The main parts were made of SUS 316 and machinable ceramic (macerite) as shown in Fig. 4. Furthermore, the ellipsoidal mesh lens was made of (#100, \(\phi_{\text{apert}}\): 50 \(\mu\)m, SUS 316) woven-mesh, which was solved in acid and pressed in a special way [24] (Fig. 4(a)).

The reason of 11 mm shifting is originated due to the fact that the present WAAEL was designed to be the part of a large Stereo-PEEM system (Fig. 5) [36] without leaving enough space for fixing of an MCP at the first focal plane (\(Z_0\)). Because the image plane was shifted in “imaging” mode the sample had to be shifted \(z=11/5\) mm closer to the mesh–lens resulting in a larger acceptance angle (\(z = \pm 65^\circ\)). For image acquisition and processing the SciLab free platform [29], with SIP Toolbox [30] was used.

![Fig. 1. Schematic drawing of Wide Acceptance Angle Electrostatic Lens (WAAEL) [21].](image1)

![Fig. 2. Design of WAAEL made using Solid Edge 3D Cad software [25].](image2)
4. Performance as an energy analyzer

4.1. Energy resolution for point source sample

The energy analysis was made using the large chromatic aberration of WAAEL at the focal plane \( z = Z_0 \), where the energy selection aperture is set as shown in Fig. 1.

In the case of our instrument for small \( \Delta E_s \) and \( \Delta Z_s \) the simulation shows that the electrons with \( E = E_0 + \Delta E \) energy focus at \( Z = Z_0 + \Delta Z \) with a relation

\[
\Delta z = 1.897 \frac{\text{mm}}{\text{eV}} \Delta \epsilon
\]

where \( E_0 = 1000 \text{ eV} \). The transmittance \( I_{\text{rel}} = I/I_0 \) for a point source of the electrons with energy \( E = E_0 + \Delta E \) as a function of \( \Delta E/E_0 \), aperture diameter \( d \) and acceptance angle of \( \pm 60^\circ \) is written as [21],

\[
I_{\text{rel}} = 1 \quad \text{if} \quad \frac{|\Delta E|}{E_0} \leq 1.24 \times 10^{-3} d \quad \text{and}
\]

\[
I_{\text{rel}} = 1.538 \times 10^{-6} \left( \frac{d^2}{(\Delta E/E_0)^2} \right) \quad \text{if} \quad \frac{\Delta E}{E_0} > 1.24 \times 10^{-3} d
\]

Fig. 1. Trajectories of several kinetic-energy electrons simulated by SIMION Ion and Electron Optics Simulator [28].

Fig. 3. (a) Mesh-lens and the first three electrodes, (b) the whole lens without deflectors and (c) the view of the whole instrument.

Fig. 4. (a) Mesh-lens and the first three electrodes, (b) the whole lens without deflectors and (c) the view of the whole instrument.

Fig. 5. Whole design of Stereo-PEEM made using Solid Edge 3D Cad software [25,36].
magnification in the case of our instrument were taken into account (Fig. 1).

Fig. 6(a) shows this transmittance for \( d = 5, 3, \) and 1 mm by dotted, dashed and solid lines, respectively. The resolving power \( \Delta E_{\text{FWHM}}/E_0 \) is defined by the full-width at the half maximum of the transmittance, which is given as

\[
\frac{\Delta E_{\text{FWHM}}}{E_0} = 3.51 \times 10^{-3} d
\]

and drawn by straight line in Fig. 6(b).

Fig. 6(b) shows that WAAEL expectedly can be used as an energy analyzer with a good energy resolution of 0.1% when the aperture diameter is 0.5 mm and the beam size is smaller than 3 \( \mu \)m as it is detailed in the next chapter. However, the transmittance curves in Fig. 6(a) show long tails, which is unavoidable in this type of focus–defocus analyzer. This long tail originates from the fact that the electron on the central axis passes the aperture even if the energy is different from \( E_0 \) as shown in Fig. 1. Hence, only a small angular region around the axis contributes to this long tail. When we cut the central small angular region, say \( \pm \beta \), the tail can be avoided. The transmittance by cutting \( \beta = 5^\circ \) and \( 10^\circ \) are shown in Fig. 6(a) by the upper part of chain-dotted and chain-double-dotted lines, respectively.

This long tail also caused serious background in DIANA when it was used without a retardation grid in electron diffraction experiments [1,31], but the retardation caused blurring of the diffraction spots, making it better not to use to observe clear diffraction patterns. In this case, the strong background obscures observation at the center (actually it was the central band instead of the central spot in DIANA). However, this problem can be partly overcome in WAAEL, because it has some kind of high-pass filter effect, so strong secondary electrons cannot pass through even at the center. Fig. 3 shows how the mesh lens works as high pass filter. Note that the electrons with an energy lower than 600 eV are repelled by the central hump and cannot contribute to the peak in the spectrum at \( E_k = 1000 \) eV, which means that this hump has some effect as a high-pass filter.

4.2. Obtained energy spectrum

We have measured the energy-resolution of WAAEL at 3 different apertures (\( d: 1, 3 \) and 5 mm) using a mesh sample (SUS316, \#250, \( \varnothing 50 \mu \)m). Fig. 7 shows the energy spectrum obtained using 1 mm aperture. The relative energy resolution was measured in one way from the whole image and another way from the intensities of a selected small region (0.2% of the whole image area) for different aperture diameters and compared with calculations (Fig. 8b) [21].

It is visible well that the point source model (Eqs. (2) and (3), solid line in Fig. 8b) cannot describe the measured data at all. The solution for the problem was obtained by making more realistic calculations taking into account the effect of emission area and position. The basic concept is shown in Fig. 9. Since the electron beam inclines to the sample surface with \( l \) (Fig. 1), the emission area becomes ellipse moreover, can be shifted in the all \( x, y \) and \( z \) directions with \( dx, dy \) and \( dz \), respectively. At the image plane, which position \( (Z=Z_0+\Delta Z) \) depends on \( \Delta E \) (Eq. (1)), the 5-times

![Fig. 6. (a) Transmittance \( I/I_0 \), (b) energy resolving power \( \Delta E_{\text{FWHM}}/E_0 \) of WAAEL in the case of point source.](image1)

![Fig. 7. Energy spectrum obtained from a selected area through 1 mm aperture. An elastic peak and plasmon-loss peak are seen.](image2)
The magnified image of the ellipse appears. Then each of the i-th point of this image can be treated as a point source and Eqs. (1)–(3) were used to get the $I/I_{\text{max}}$ ratio and the resolving power. Each of these i-th point source forms cone with an angle of $2\alpha/5$ and intensity ($I_i$) and is cut by the aperture hole contributing to the measured intensity with $I_{\text{meas}}$. The $I_{\text{meas}}/I_i$ ratios for different energy electrons and the integral for the whole image area were determined using Monte Carlo Simulation. The result is shown in Fig. 8a. Although we could not describe the measured data quantitatively (maybe some parameter were not taken into account i.e. the sample was mesh and not solid, etc.) the calculated results qualitatively agree with the measured ones. It is worthy to see how the changes in the sample area and position can influence the energy resolution of an aperture filtered electron spectrometer.

5. Performance as an electron emission microscope

5.1. Lateral spatial resolution

The spatial resolution of WAAEL is limited by the: (1) spherical aberration that can be decreased by the design, the (2) fabrication accuracy, (3) mesh-hole effect, and finally the (4) chromatic aberration. For monochromatic rays the spherical aberration is defined by the focusing spot size for the electrons emitted from one point on the optical axis. Without taking into account the lens effect of mesh-holes, the spot size can be made as small as it is wanted by modifying the shape of the ellipsoidal mesh as well as, adjusting the shape and voltages of the electrodes [18]. However, the accuracy of the simulation software is limited by the applied step size and also the fabrication tolerance to be around 1 $\mu$m. Hence, at this stage the focusing spot size is limited to be around 1 $\mu$m due to the above effect of (1) and (2). In the following section, we will discuss the effects of (3) and (4).

5.2. Mesh-hole effect

Although, the distortion of the electric field around the small mesh-hole blurs the focusing spot size up to about the size of the mesh-hole [32], where the spot size was estimated using the Davison–Calbick formula [33,34], we were able to measure a lateral resolution of 27(4) $\mu$m using a mesh with 250 $\mu$m hole diameter as it is shown in the following section. Hence the limit of the lateral resolution can be estimated to be around some $\mu$m when one uses 40 $\mu$m diameter hole-size mesh, which is currently under construction.
5.3. Chromatic aberration and diffraction limit

The chromatic aberration also limits the lateral resolution and can be calculated easily for a point source. The energy resolution of present WAAEL can be 0.1% or less, as described before. The chromatic aberration disc diameter \( d_c \) at the focal plane as a function of acceptance angle \( \alpha \) and \( \Delta E/E_0 \) can be written as [21]

\[
dc = \frac{758.8 \, \tan(\frac{\alpha}{2}) \; \Delta E}{E_0} \quad [\text{mm}]
\]

and plotted in Fig. 10 for \( \Delta E/E_0 = 10^{-3} \) and \( 10^{-4} \) as a function of \( \alpha \).

The diffraction limit can then be given by the diameter of Airy disc \( d_{\text{Airy}} \) [21]

\[
d_{\text{Airy}} = 2 \cdot \frac{0.61 \lambda}{\sin \alpha} = \frac{4.71 \times 10^{-8}}{\sin \alpha} \quad [\text{mm}].
\]

Calculating with e.g. \( \alpha = 60^\circ \) and \( \Delta E/E_0 = 10^{-3} \) the chromatic aberration disc diameter is \( d_c = 161 \, \mu\text{m} \) or, with \( \Delta E/E_0 = 10^{-4} \) \( d_c = 16 \, \mu\text{m} \), which are much larger than the diffraction limit. Hence \( \Delta E/E_0 = 10^{-5} \) is necessary to obtain about 1 \( \mu\text{m} \) lateral resolution for this system.

5.4. Obtained image

Although, the aperture is the only energy filter in the present system and the fabrication accuracy of our first version ellipsoidal mesh lens was not better than 0.05 mm, we could see 5-times magnified images with 27(4) \( \mu\text{m} \) lateral resolutions as follows. To see an image with this first system without energy selector, it was easier to take images outside of the central zone, where the background is lower, or to apply certain background subtraction techniques. In these measurements, we used the elastic peak \( E_e = E_0 = 1 \, \text{keV} \) for imaging.

Fig. 11 shows one of the rough images of a mesh sample (SUS316 #250, \( \varnothing_{\text{wire}} = 30 \, \mu\text{m} \), \( \varnothing_{\text{aperture}} = 3 \, \text{mm} \)) without background subtraction. We were able to obtain it by locating the emission area out of the axis (Fig. 11(a)) then shifts the image back to the center by deflectors (Fig. 11(b) and (c)). The deflector influences the lower energy electrons more strongly than the elastic ones, producing slight energy filtering effect.

For testing the lateral resolution of our lens we investigated mesh samples with various densities. The upper right corner of

![Fig. 11](image1.png)

Fig. 11. Images of the mesh sample on the screen. Deflector and 3 mm aperture were used as energy filter. (a) Image when the irradiated region is off-axis. (b) and (c) The image of the mesh sample was shifted towards the center by a deflector.

![Fig. 12](image2.png)

Fig. 12. Image of SUS316 #400 mesh with \( \varnothing_{\text{wire}} = 30 \, \mu\text{m} \) and its intensity distribution taken through 5 mm aperture (\( \alpha = 60^\circ \)). The dots are measured data, the line is fitted Gaussian convolved with a wire related square wave function.

![Fig. 13](image3.png)

Fig. 13. One of the images of the translational video of a mesh sample (SUS316, #250, \( \varnothing_{\text{wire}} = 30 \, \mu\text{m} \)) (a) before and (b) after background subtraction by sigma-clipping method.

Fig. 12 shows an image of SUS316 #400 mesh (wire spacing is 63.5 \( \mu\text{m} \), with \( \varnothing_{\text{wire}} = 30 \, \mu\text{m} \)) taken through 5 mm aperture. The reason why the horizontal lines are not visible is that the incident angle of electron beam was lower here than in other cases. The horizontal intensity distribution was fitted with Gaussian functions. The fitting resulted of 33(3) \( \mu\text{m} \) FWHM for the measured peaks that were deconvoluted with a square wave function representing the sample to obtain finally the lateral-resolution of our lens as \( \sim 27(4) \, \mu\text{m} \) FWHM. This result is about ten times better than that was predicted by the mesh-hole blurring effect and the chromatic aberration disc size, but far from the \( \sim 4 \, \mu\text{m} \) resolution engaged by the MCP (the diameter of the envelope of three 10 \( \mu\text{m} \) diameter MCP cell) and the 5-times magnification of the MCP. The resolution limit originated from the accuracy of simulation and fabrication processes. Our next ongoing task is to improve the quality of fabrication reaching about 1 \( \mu\text{m} \) resolution.

![Fig. 10](image4.png)

Fig. 10. Calculated lateral resolution in the case of point source.
The quality of the measured image can be improved by distinguishing the background from the real image and then subtracting that. Therefore, the best way is to take a series of photos where the background and the images behave in a different, but known way.

One of these methods is to utilize the fact that the image of the sample moves, but the background does not move at the same time. Then one can try to distinguish the steady background or isolate the moving structures on different pictures. We have chosen to apply the first, simpler method. The images were averaged after subtracting pixels with standard deviations greater than certain values for all images (Fig. 13). This method is iterative and called sigma-clipping [35].

Another method to distinguish the background from the image is to take spectral images at several pass-energies and subtract the background estimated by Shirley algorithm (Fig. 14). This kind of background subtraction can make the image visible even at the lens axes where it cannot be observed without energy filtering. We have tried this method in two different ways. The first was the dot by dot method where the Shirley-background (\( I_{\text{Shirley}}(E,x,y) \)) was calculated by applying the iteration for the same \( x \) and \( y \) coordinate pixels through all different energy (\( E \)) images and then subtracted from the spectra (\( I(E,x,y) \)) resulting background-free images (\( I_{\text{Sub}}(E,x,y) \) ) (Eq. (6), Fig. 14).

\[
I_{\text{Sub}}(E,x,y) = I(E,x,y) - I_{\text{Shirley}}(E,x,y).
\]  

This method results in clear and detailed images, but requires very long calculation time for usual PC-s. Therefore, we have tried it just for small size and small number of images where neither the lateral nor the energy resolution is sufficient.

However, one can decrease the calculation time by calculating and subtracting not the dot by dot Shirley-background, but the total Shirley-background normalized to the first and last images (\( I_{\text{Shirley\_norm}}(E,x,y) \) ) (Eqs. (7)–(10)). Although, we lose information by this method compared to the first one (Eq. (6)), but less time is needed to achieve relatively good results.

\[
I(E) = \sum_{x,y} I(E,x,y)
\]  

\[
N(E) = \frac{I_{\text{Shirley}}(E) - I_{\text{Shirley}}(E_{\text{max}})}{I_{\text{Shirley}}(E_{\text{min}}) - I_{\text{Shirley}}(E_{\text{max}})}
\]  

\[
I_{\text{Shirley\_norm}}(E,x,y) = \frac{I(E_{\text{max}},x,y) + N(E)(I(E_{\text{min}},x,y) - I(E_{\text{max}},x,y))}{I(E_{\text{max}},x,y) - I(E_{\text{min}},x,y)}
\]  

\[
I_{\text{Sub}}(E,x,y) = I(E,x,y) - I_{\text{Shirley\_norm}}(E,x,y).\]

These methods are not just useful for producing better quality images, but can be used to obtain more information from the measured data i.e. the image can be seen even in the optical axes at the center of the screen (Fig. 15) without energy filtering.

Furthermore, it was very helpful in perfecting the design as well as, structure and parameter settings of WAAEL during the
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Fig. 16. LEED pattern of MgO crystal taken at 80 eV electron energy.

first testing process. In this way, we were able to get better spatial resolution without using additional energy filter other than the aperture.

6. Performance as a two-dimensional angular distribution (TDAD) analyzer

Beyond the above mentioned results two-dimensional angular distributions were measured using a 0.24 mm aperture. An example LEED pattern is shown in Fig. 16, from MgO crystal taken at 80 eV electron energy where the clearly visible five spots show the capability of our prototype lens for angular distribution measurements.

7. Conclusion

We have designed, built and tested successfully a new wide acceptance angle electrostatic lens, which achieves its calculated capabilities and opens new ways for highly sensitive analyzers simultaneouse angular distribution measurements from a seletected area, and photoemission electron microscopes (PEEM). In the near future, this instrument will be extended with an additional lens system and energy analyzer and will be applied as a new type Stereo-PEEM [36].