



Optimization strategy for retardation potentials in a photoelectron time-of-flight spectrometer

Edyta Osika

AGH University of Science and Technology, Cracow, Poland

Supervisor: Jens Buck

7 September 2011

Abstract

The aim of this project was to establish strategy for optimizing performance of a photoelectron time-of-flight spectrometer. Parameters tuned while optimization were retardation potentials on spectrometer's electrodes. Two types of strategy have been introduced. For one of them actual results are shown, for the second one experimental examinations have been carried out and are described in this paper. Both strategies are meant to complement one another and provide well-defined way to improve performance of considered device up to its limits.

Contents

1	Introduction	3
2	Strategies of optimization	5
2.1	First strategy: simulations	5
2.1.1	Method	5
2.1.2	Results	6
2.2	Second strategy: one-dimensional model	9
2.2.1	Method	9
2.2.2	Experimental data	11
3	Conclusions	14
4	Acknowledgements	14

1 Introduction

It is an indisputable fact that X-ray sources are of great importance for many fields of nowadays science. Improving brilliance of these facilities is a driving force for further research and development. The latest project of such source - the European XFEL (X-Ray Free Electron Laser) - can establish a new outstanding achievement in providing the highest quality radiation. Completion of the project is expected to take place in 2015.

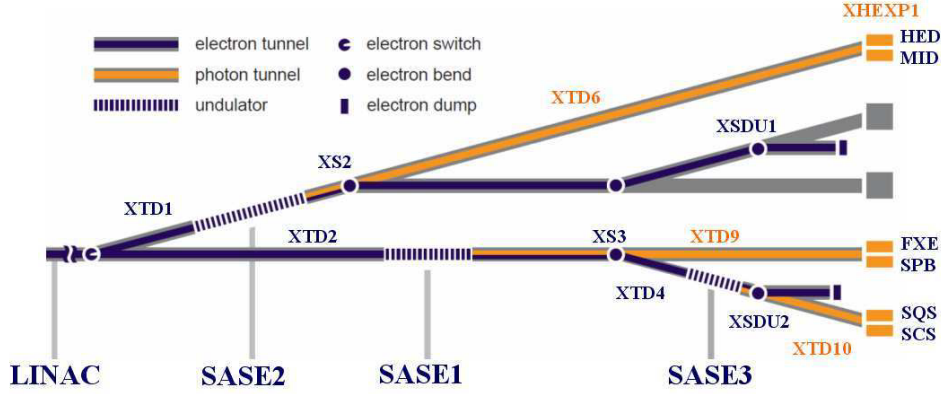


Figure 1: General layout of the European XFEL's lines.

For proper analysis of results of many experiments planned to be held at XFEL precise knowledge of photon beam's parameters is indispensable. That refers to photon energy as well. Ranges of energy available for specific SASE lines are expected to be: 0.28 - 3 keV for SASE3 and 3 - 25 keV for SASE1 and SASE2 and spectral bandwidth of radiation in both cases on the order of 10^{-3} . The wavelength stability is predicted to be on the order of 1%, but a relative precision of energy measurement of at least 0.1% should be obtained. For these reasons - information for scientists and constant monitoring of possible energy fluctuations - there is a need of online device, which can measure photon energy during facility's operation and not consume the beam in the same time. One of candidates for meeting these requirements is gas based photoelectron time-of-flight spectrometer. But to determine if obtaining desired resolution with such device is possible and, in case, to improve its performance some systematic strategy of optimization is necessary.

Possible usage of eTOF spectrometer for XFEL is currently investigated in WP74 (Work Package 74: X-ray photon diagnostics). Design of spectrometer now being under consideration has been developed in group P04 at PETRA. It consists of 16 flight tubes disposed radially, perpendicular to the beam. As can be seen on Figure 2 each tube includes 5 electrodes: 3 cones, 1 cylinder and mesh at the end of the tube. The mesh is electrically connected to the cylinder, so potentials on both are always the same. Behind the mesh a MCP (micro-channel plate) stack, a capacitor and electronics (acquiring and amplifying the signal) are situated. The inner ring of the spectrometer also works as an

electrode, so in result one has 5 degrees of freedom for defining electric field inside all flight tubes and beamline. Symmetry of spectrometer and number of flight tubes allow to use the device for measuring not only energy but polarisation of light as well.

Optimization considered in this paper regards tuning voltages on all electrodes this way to obtain the best performance of the setup. This task is not as straightforward as it may seem, because one has to take into account many different aspects of measurement procedure and results. The most important parameter of the spectrometer to focus on is energy resolution - the main goal of the device in general is to achieve precision of measurement as mentioned in the text above. Nevertheless one can not forget about other important issues like transmission, reasonable time-of-flight values or signal-to-noise ratio. Transmission is particularly important here, because for high energies as those available in XFEL, cross section for photoionization is very low (even for the most appropriate gases like, planned to be used, Xe, Kr) and therefore the expected signal is low. Additionally, the device is supposed to gain complete data for every single pulse of light which duration is of the order of 10 femtoseconds. And finally we are limited by opening angle of flight tubes of about $5 \cdot 10^{-3}$ of 4π .

That claims for special care of every photoelectron created. For the same reason rather homogenous coverage of the detector is desired - not to lose any signal during MCP channels' dead time. As for reasonable time-of-flight values large retardation potentials are necessary to slow down high energetic (up to 10 keV) photoelectrons. In the same time to prevent from overlapping of signals from different pulses, it must not exceed above time window between the pulses, which is 220 ns.

All these aspects should be taken into consideration while optimizing setup and that way measures for good or bad behaviour of spectrometer can be specified. Concerning that, strategy for optimization performance of setup by tuning retardation potentials on electrodes is presented in this paper. This strategy consists of 2 different approaches which are shown to be useful on consecutive optimization phases and finally complete each other.

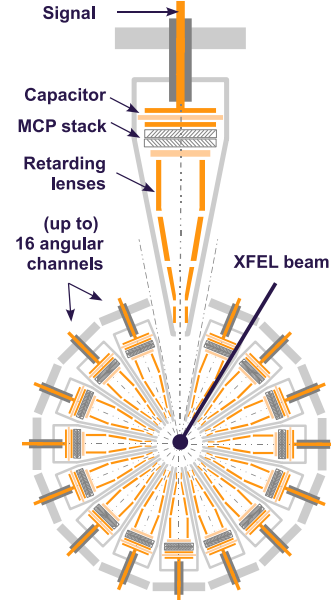


Figure 2: Scheme of a eTOF spectrometer designed in a group P04 at PETRA.

2 Strategies of optimization

2.1 First strategy: simulations

2.1.1 Method

First strategy of optimization discussed in this chapter is based on simulations carried out with SimION and code in MATLAB developed by Jens Buck. SimION is a program which provides information about particles' trajectories for specified starting conditions and voltages on the electrodes. Results of such simulations are mainly sketches of trajectories for investigated cases, as on Figure 3. Notation of voltages on electrodes is in a convention: [inner ring , 1st cone , 2nd cone , 3rd cone , cylinder and mesh].

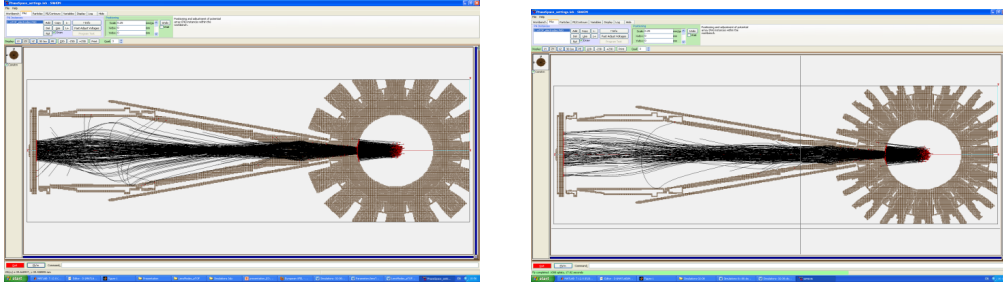


Figure 3: SimION simulations for voltages set: [0V -20V -80V -40V -98V] and [0V 10V -70V -92V -99V], electron energy 100 eV.

With analysis of these sketches one can gain general information if setting gives 'good' results - but only for transmission and noise caused by electrons hitting walls. SimION can provide also actual data for particles' starting points and points of collision and this data is exploited by MATLAB code. Program creates set of points in 6-dimensional parametric space for using as a starting conditions of particles. 6 dimensions stand for 6 degrees of freedom of single electron: kinetic energy, coordinates x, y, z, and 2 angles, ϕ and θ , (with respect to symmetry axis of flight tube) of velocity vector. This set of starting points covers whole possible range (e.g. all coordinates inside the inner ring) and is analyzed in SimION for all important parameters in points of collision. Such data can be finally used to compare behaviour of many voltages settings in a meaning of resolution. This software gives us a straightforward way for finding settings with improving resolution, however it is very time-consuming and at current stage of code's development does not yet provide absolute values for resolution, transmission or coverage of detector. That is why some measures of resolution had to be invented to compare settings properly.

2.1.2 Results

By picking 'good-looking' results from sketches of trajectories and then using them as starting points for optimization with MATLAB code, significant improvement in resolution has been possible to achieve. That can be shown on Figure 4. First pair of plots present results for one of starting points used for simulations, second for one of the best setting found during systematic investigations. Trajectories for those 2 cases are shown on Figure 3. The second setting can be considered as a candidate for experimental examination. For measure of resolution we were using degree of overlap of peaks at time-of-flight histograms. Histograms contain all time-of-flights for simulated photoelectrons for small ranges of their initial kinetic energy. Plots displaying intervals, where centre 68.2% of data points are distributed, provide information how easy to distinguish are neighbouring peaks by defining position of their 0.159 and 0.841 quantiles. This interval is equivalent to FWHM interval for normal distribution, but due to asymmetric shape of peaks fitting Gaussian distribution would not be appropriate here.

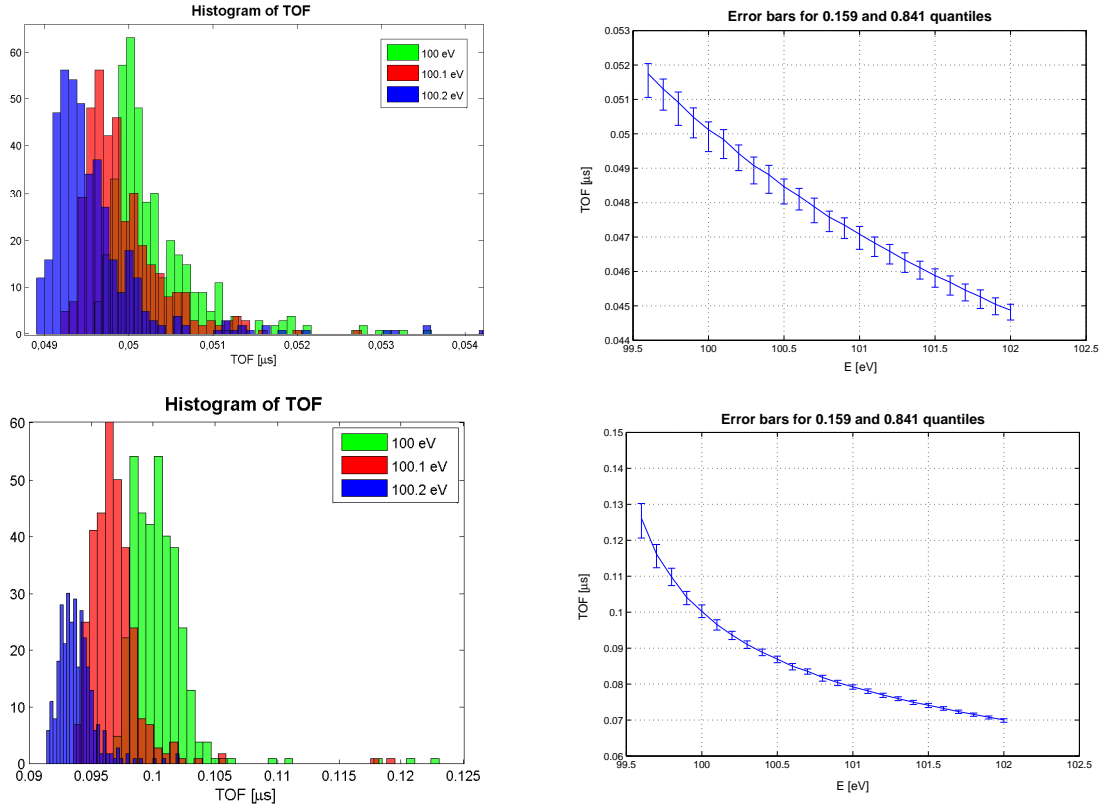


Figure 4: Results for settings: [0V -20V -80V -40V -98V] and [0V 10V -70V -92V -99V], electron energy 100 eV.

This method does not provide any measure of real energy resolution but even though

the data has a potential because gives reliable comparison between settings. We can not tell with these simulations how good one particular setting is, but we can demonstrate that one is better than others.

For the best setting found (mentioned before) there is easy way to move comparable 'resolution' to higher energies. Cases examined for 100 eV has been shifted to 250 eV and 500 eV by proportional increase of potentials of 2nd and 3rd cone, slightly tuned proportional increase on the cylinder and leaving the same voltages on inner ring and 1st cone. Results are shown on Figure 5.

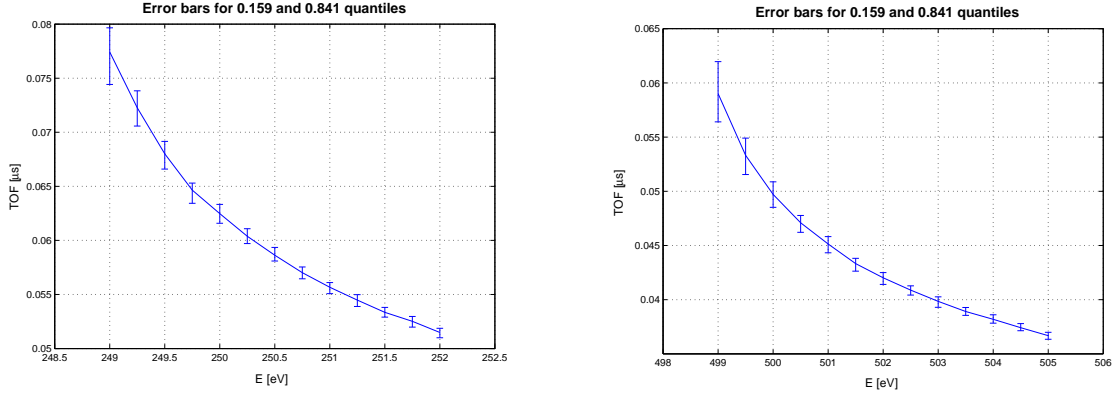


Figure 5: Results for settings: [0V 10V -175V -230V -248V], electron energy 250 eV and [0V 10V -350V -460V -497V], electron energy 500 eV.

Good prediction for those results gives comparison with rule of thumb currently in use in group P04 at PETRA. This rule is already effective and simulations show that considered setting probably might work even better. Plot of errorbars for rule of thumb (for electrons energy 500 eV) is presented on Figure 6 and can be compared with those presented before. Values for potentials on electrodes stand for percentage of electron's energy used as retarding potential.

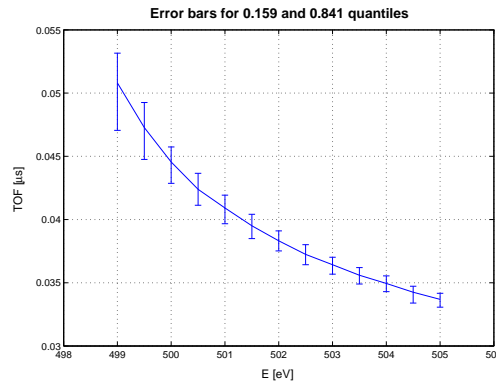


Figure 6: Rule of thumb: [0V -65% 0V -90% -100%], electron energy 500 eV.

Such simulations as presented above are good strategy for gaining interesting settings to examine with experiment. Weak point of this method of optimization is fact that simulations usually take a long time and we are therefore limited to investigate only small discrete collection of settings. However the second strategy of optimization can be developed with one-dimensional model, which is described in next chapter. If second strategy will occur reliable, the first one would not need to provide us ultimate settings but only candidates for further investigation.

Apart from finding reasonable starting points for one-dimensional model, simulations carried out provided few general conclusions for optimization of considered spectrometer:

- hint for further simulations with SimION: the best results for resolution were given by all electrons' trajectories kept near the symmetry axis of flight-tube (at least in region of 3 cones),
- large retardation potential on the cylinder (about 98-99% of electrons kinetic energy) is essential to shift examined energy to steeper part of TOF/Energy curve and obtain better resolution.
- keeping 0V on inner ring and positive potential on 1st cone in simulated cases works well for resolution and could contribute to attracting electrons and repelling ions. This particular effect might be strongly desired for preventing ions from getting into flight tubes and producing background for proper signal.

2.2 Second strategy: one-dimensional model

2.2.1 Method

As was mentioned before, simulations conducted with SimION and MATLAB code seem reliable but are also very slow. That is why looking for the limit of spectrometer's performance might take unreasonably long time and that is way faster strategy is required. For this reason idea and implementation of one-dimensional model were developed by Jens Buck. The model, using potential arrays from SimION and special MATLAB program, analyses flights of particles only exactly on symmetry axis of flight tube. Due to rotational symmetry of tube these particles are captive on one axis and can be considered as points in one-dimensional space. Taking advantage of that, one can gain better control of some specific parameters in TOF/energy dependency, like: initial kinetic energy, total time of flight or dispersion (first derivative of TOF/energy curve). The model is able to provide new sets of voltages (continuously changing) for chosen parameters nearly constant. Example of plots delivering new voltage settings is shown on Figure 7.

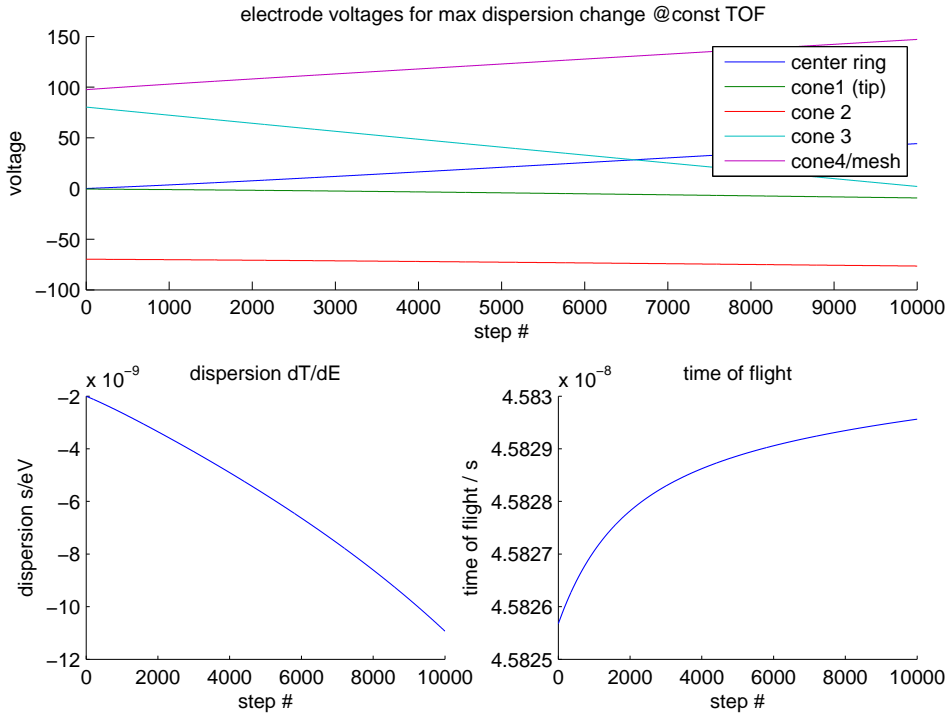


Figure 7: Changing dispersion at constant TOF and energy for starting point : [0V 0.52V 69.74V -80.34V -97.54V], electron energy 104.4 eV .

One-dimensional model is a strong simplification of the problem, which is though very efficient to compute. If results are representative for all electrons, had to be examined and such examination was a main purpose of experiment held in the end of August 2011 at BW3 beamline at DORIS.

Strategy derived from one-dimensional model is independent of setup examined. In experiment we used simplified spectrometer, instead of 16 tubes consisting only of 2 on opposite sides of the beamline. It can be also considered as representation of complete array of detectors.

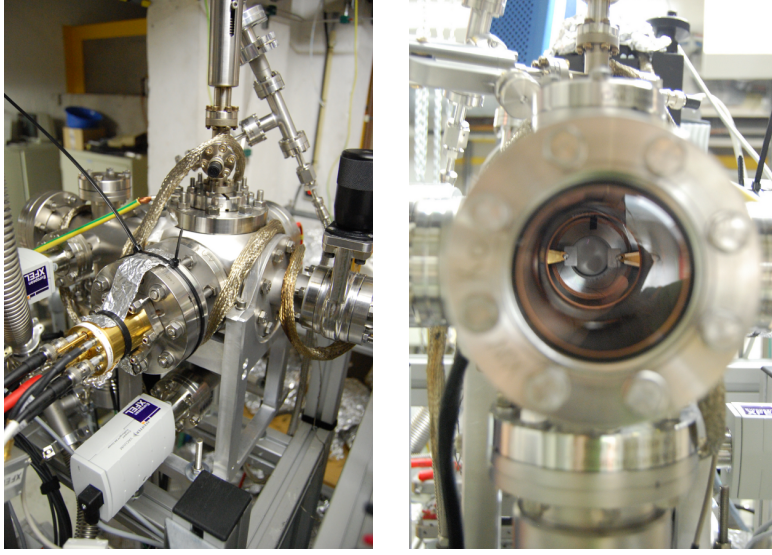


Figure 8: Experimental setup: (1) Chamber with housing of one of flight tubes visible. (2) Insight into the chamber.

As gas for photoionization we used Neon, and spectrum acquired is corresponding to its absorption edge 21.6 eV. During the experiment, vacuum in the chamber was kept on the level of approximately 10^{-6} mbar. Energy of photons for gained spectra: 123 eV. Very important thing to consider during measurements is that one-dimensional model does not give results for the mean value in TOF(time of flight)/energy dependency but for supporting curve, like on Figure 9.

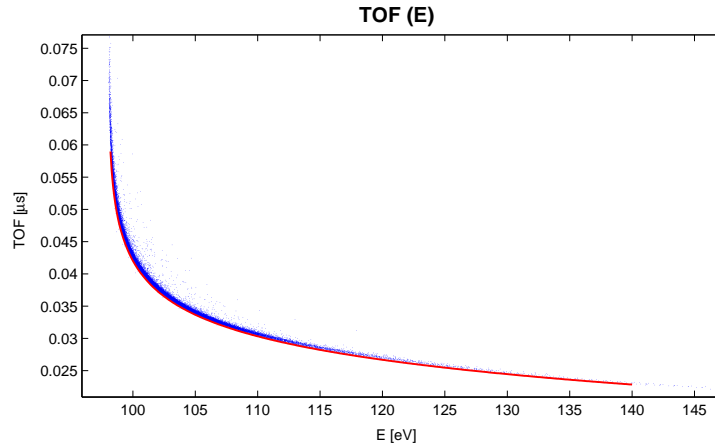


Figure 9: Comparison of TOF/energy dependency for one-dimensional model and simulations for whole parametric space.

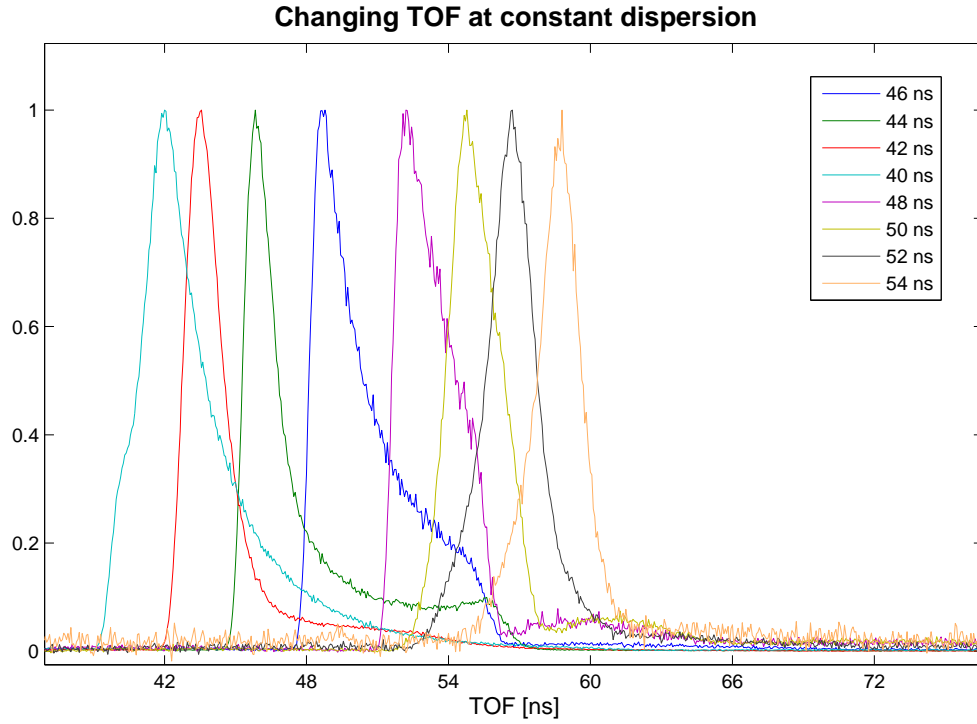
Blue curve is simulated for particles from whole reasonable parametric volume and red curve for particles exactly on symmetry axis. Difference between plots suggests that thinking of time of flight in model should be replaced by thinking of the shortest time of flight measured. In practice that means considering not the highest point of spectrum's peak but its onset.

2.2.2 Experimental data

Among data acquired during experiment, 3 sets of spectra are most interesting and provide some evaluation for one-dimensional models efficiency. These measurements were carried out for modes:

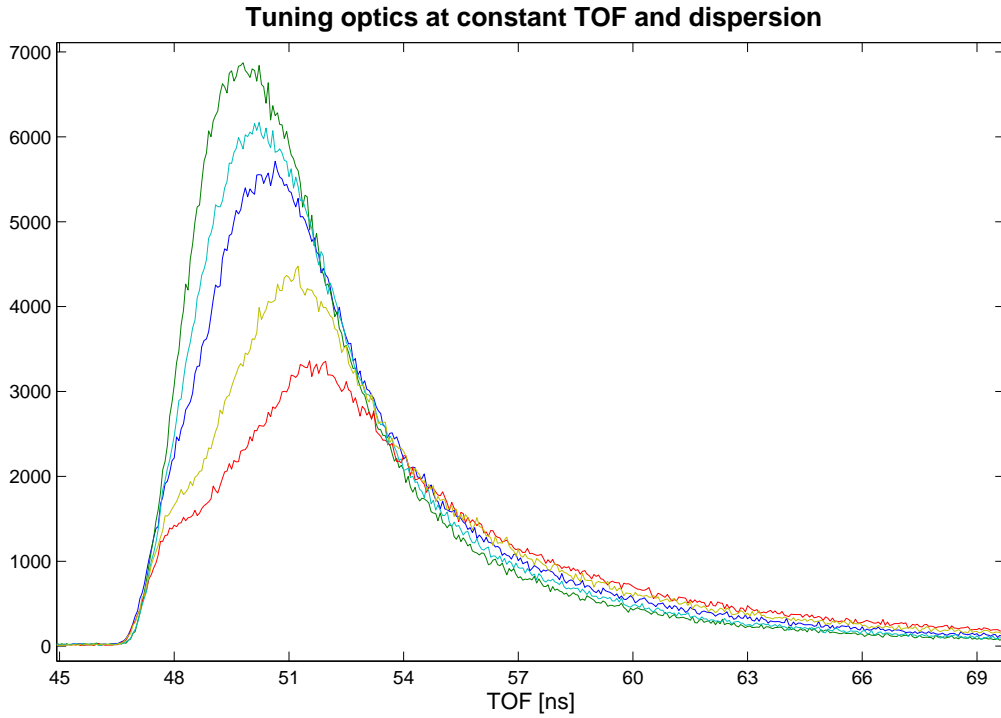
- changing TOF at constant energy and dispersion,
- keeping all - TOF, energy and dispersion - constant and tuning only optics,
- changing dispersion at constant energy and TOF.

Results are commented below.



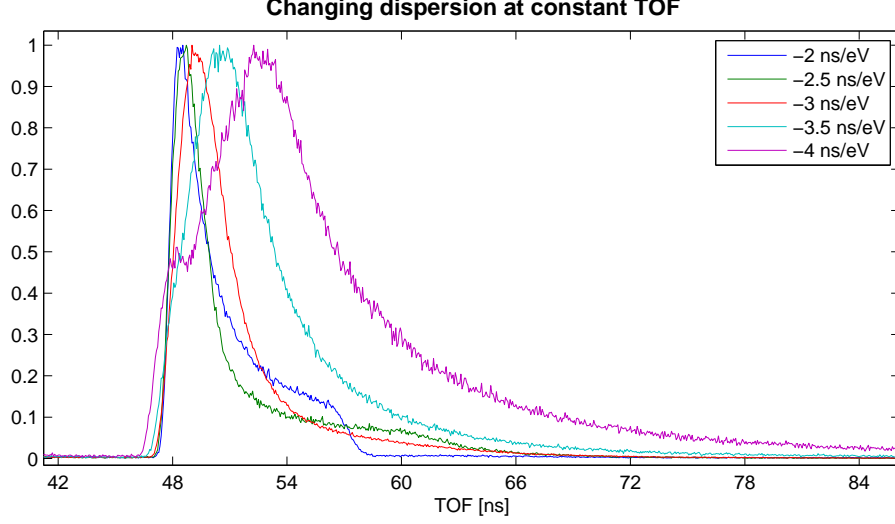
Measurements for first mode (changing TOF at constant energy and dispersion) showed that concept of considering onset instead of TOF works very good. On the plot there are 8 spectra presented for TOF systematically being changed at other parameters constant. In every spectra constant background was removed. All spectra are also normalized to a maximum of 1, just to make discussed feature more visible. In the table theoretical TOFs from one-dimensional model are compared with actual experimentally obtained onsets. Relative errors for onset and TOF for all spectra are rather small - on order of few percents. This means that one-dimensional model really allows to control at least one of parameters - onset of the peak. The exact values are in this case not the most important, but it's sufficient that tendency of changes is exactly as expected.

Onset [ns]	Theoretical TOF [ns]	Relative error
39.3	40	1.8%
42.06	42	0.1%
44.64	44	1.5%
47.58	46	3.4%
51	48	6.3%
52.08	50	4.2%
52.38	52	0.7%
54.48	54	0.9%



The second mode we acquired data for is keeping all parameters constant and tuning only optics. This mode could be particularly useful during next experiments because it should allow to gain better transmission without changing general parameters of spectrum. In

data presented we are going in wrong direction - from green to red curve so to lower transmission - but still it demonstrates power of the model by keeping onset almost perfectly constant.



The last spectra were collected using third mode - changing only dispersion at other parameters constant. Utility of this mode could be very meaningful because dispersion currently has the biggest influence on peak's width and resolution.

Stability of onset can again be regarded as a proof of proper operation of one-dimensional model. In this case we should consider change of peak's width really as an effect of changing dispersion. Actual numbers are inserted into table and from this information we can calculate relative changes of quantities included. As an approximate measure of dispersion we can treat FWHM of peaks. For relative change of theoretical dispersion equal 100% we gain increase of FWHM equal 263%. But why peaks

Dispersion [ns/eV]	FWHM [ns]	Onset [ns]
-2	2.1	47.10
-2.5	2.1	47.04
-3	3.0	46.92
-3.5	4.92	46.62
-4	7.62	46.26

are so much wider? As was said one-dimensional model considers only supporting curve for TOF/energy dependency. That is why behaviour of all particles not on tube's symmetry axis is too unpredictable to determine exact shape of peak without examination. Anyway these spectra clearly show that with discussed model we are able to effectively control changes of dispersion at constant onset and energy.

3 Conclusions

Experimental data shows that one-dimensional model gives expected results in practical use and allows to tune important for resolution quantities in predictable way. This strategy of optimization is also very fast so can be indispensable for use during experiment. However, it explores only specified neighbourhood of starting voltage setting so possible improvement might be this way limited. Still reasonable starting points for examining with one-dimensional model can be provided by simulations with SimION and MATLAB code. Thus both strategies considered in this paper can complement one another and form complete method of optimization. Additionally this strategy should not be limited by current design of spectrometer, but should be useful for any other spectrometer of similar symmetry.

4 Acknowledgements

I would like to thank my supervisor Jens Buck for constant invaluable support he has been giving to me, as well as for his knowledge and experience, which he never refused to share. I would like to thank also Jan Grünert and Cigdem Ozkan for help and good advice always when I needed it. And finally I would like to express my gratefulness for whole P04 group at PETRA, who presented us with their beamtime, allowed to use their setup and, as if that would't be enough, gave support even during experiment!

References

- [1] European XFEL Technical Design Report, 2006
- [2] website: www.epn-campus.eu/uploads/media/06.BUCK.01.pdf
- [3] Conceptual Design Report: Scientific Instrument SQS, M. Meyer
- [4] Layout of the X-Ray Systems at the European XFEL, Th. Tschentscher