Summerstudent report

Optimization of voltages for spatial map imaging and velocity map imaging

Miguel Ángel Martínez García

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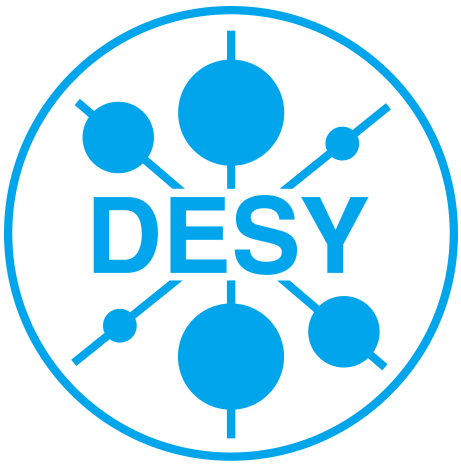

Supervisor: Sebastian Trippel
Center for Free-Electron Laser Science (CFEL)
Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Abstract

In this work we have determined the best voltages for working with spatial map imaging and velocity map imaging. We have computed them combining simulations in SIMION with Taylor approximations. Furthemore we have calculated the velocity of the molecular beam for a given temperature in the lab combining experimental results and simulations.

Contents

1 Introduction

The last years have seen how velocity map imaging[1] (VMI) have been useful for chemical reaction dynamics, photoelectron spectroscopy, molecules in strong laser fields, pump-probe spectroscopy and photodissociation. This mode projects the velocity coordinates given in a interaction region on the detector as spatial coordinates. To get it, we use electrostatic lens, which are electrodes with a difference of potential between them.

On the other hand, spatial map imaging (SMI) is useful for biomedical imaging, studying laser beam profiles or map spectrometry. In this case, this mode projects spatial coordinates in the interaction region on spatial coordinates in the detector.

The main goal of this work was to implementate a Taylor approximation method to find the optimized voltages for each mode [3].

2 Experimental setup

The experimental setup is presented in the figure below.

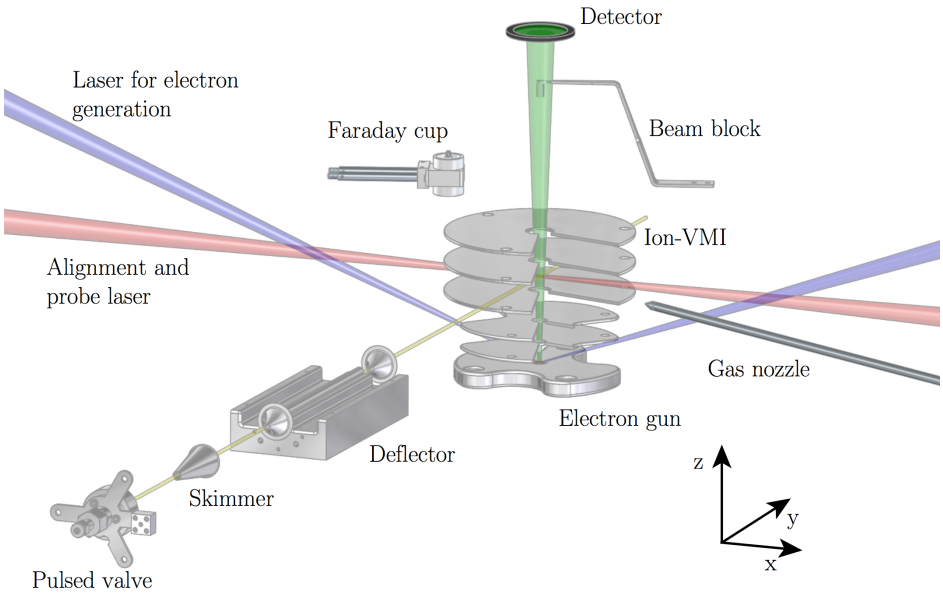

Figure 1: Experimental setup [4]

There are six electrodes, the first three are for electron difraction experiments, so we only used the other three electrodes which are to acelerate ions acting as electroctatic lens. The molecular beam is generated by a pulsed valvue and it is perpendicular to the lens direction. The gas pass three skimers until getting the interaction region, between the first and the second ion electrodes. A laser, which is perpendicular as to the lens direction as to the molecular beam, interacts with the molecular beam generating ions by photodissociation. Then, the ions are accelerated by the electrodes stated above. Finally, the ions colisionate on the detector, and we take the messaurements with a camera which is pointing to the detector.

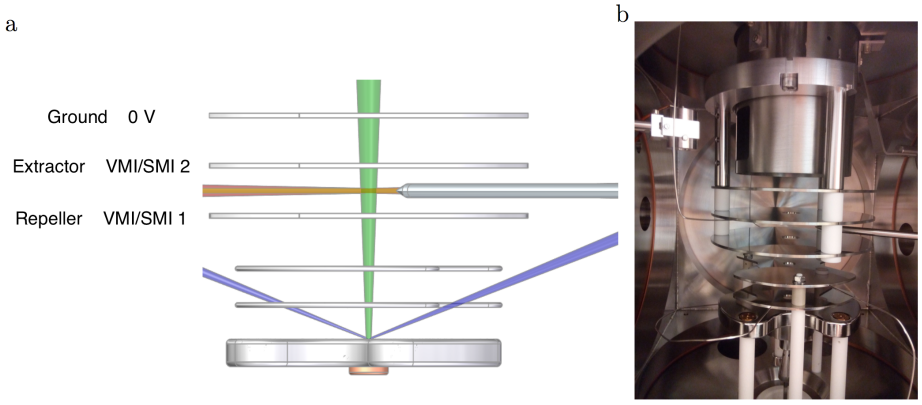

Figure 2: (a) The typical voltages for the repeller and the extractor are defined depending on if we are in VMI or SMI approach. (b) The electrodes in the lab including more elements [4]

3 SIMION 8.1

We have used the simulator SIMION. Given a electrodes configuration and the initial conditions for several ions as input, SIMION gives as output several variables which characterize the trajectories. In our case we took the Time of flight (TOF), the position and the velocities of each particle at the beginning and at the collision time.

4 Taylor expansion approach

We aproximate the imagen modes (VMI/SMI) via a Taylor aproximation. Taking X as a scalar variable of the particle at the collision time, we can approximate it with the following Taylor expansion.

$$X \approx D_X^1|_0 \begin{pmatrix} y \\ v_y \\ x \\ v_x \end{pmatrix} + \frac{1}{2} \begin{pmatrix} y \\ v_y \\ x \\ v_x \end{pmatrix}^T D_X^2|_0 \begin{pmatrix} y \\ v_y \\ x \\ v_x \end{pmatrix} \tag{4.1}$$

where

$$D_X^1 = \begin{pmatrix} \partial X/\partial y \\ \partial X/\partial v_y \\ \partial X/\partial x \\ \partial X/\partial v_x \end{pmatrix} \tag{4.2}$$

and

$$D_X^2 = \begin{pmatrix} \partial^2 X/\partial y \partial y & \partial^2 X/\partial y \partial v_y & \partial^2 X/\partial y \partial x & \partial^2 X/\partial y \partial v_x \\ \partial^2 X/\partial v_y \partial y & \partial^2 X/\partial v_y \partial v_y & \partial^2 X/\partial v_y \partial x & \partial^2 X/\partial v_y \partial v_x \\ \partial^2 X/\partial x \partial y & \partial^2 X/\partial x \partial v_y & \partial^2 X/\partial x \partial x & \partial^2 X/\partial x \partial v_x \\ \partial^2 X/\partial v_x \partial y & \partial^2 X/\partial v_x \partial v_y & \partial^2 X/\partial v_x \partial x & \partial^2 X/\partial v_x \partial v_x \end{pmatrix} \tag{4.3}$$

correspond to the first and the second order of approximation respectively. We have been able to find these coefficients making a program which analyzed and treated the results of the simulations of SIMION, obtaining the optimized voltages for each mode (VMI/SMI). The analized variables on the detector are Y and T.

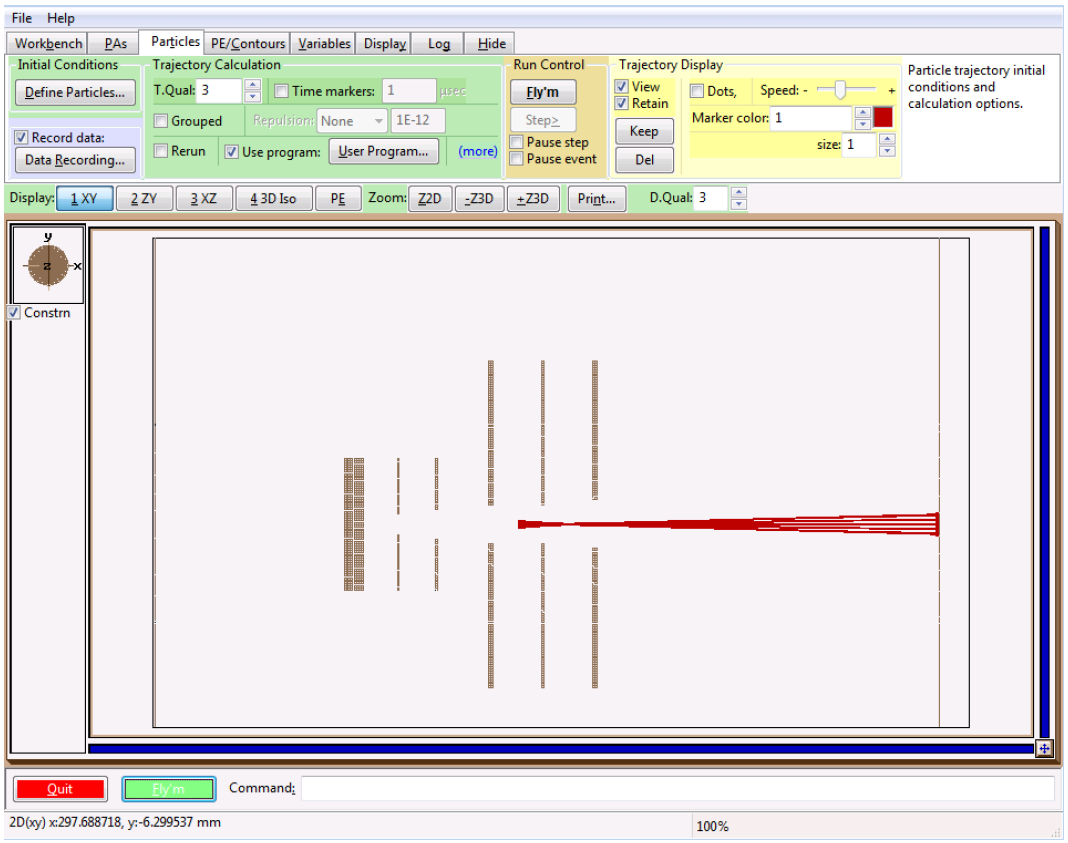

Figure 3: Example using SIMION with our setup configuration. This simulation belongs to the next section.

4.1 VMI mode

The results for the VMI mode are presented below, finally the best voltages were $V_1 = 3000\,\mathrm{V}$ and $V_2 = 1995\,\mathrm{V}$. In Figure 4 we can observe that for the coordinate Y there is only a strong dependency on v_y, while for T it is on x. It looks that in both cases the first approximation (first derivative) should be good. The coefficients for the first and the second order are presented below.

$$D^1_Y|_0 = \begin{pmatrix} -0.0012 \\ 1.8902 \\ 0 \\ 0 \end{pmatrix} \qquad D^2_Y|_0 = \begin{pmatrix} 0 & 0 & 0.0356 & 0 \\ 0 & 0 & 0.0116 & 0 \\ 0.0356 & 0.0116 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.4}$$

$$D^1_T|_0 = \begin{pmatrix} 0 \\ 0 \\ 0.0045 \\ 0 \end{pmatrix} \qquad D^2_T|_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0.0007 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.5}$$

We can observe that the vertical coordinate on the detector Y depends on v_y, as we expected for a velocity map imagin mode, and briefly on y. The last should be only due to the change which v_y provokes in y. The rest of the coefficients are zero for the first order. For the second order, almost all the coefficients are zero. It is destacable the zero which correspond to the second element of the diagonal, which means that the

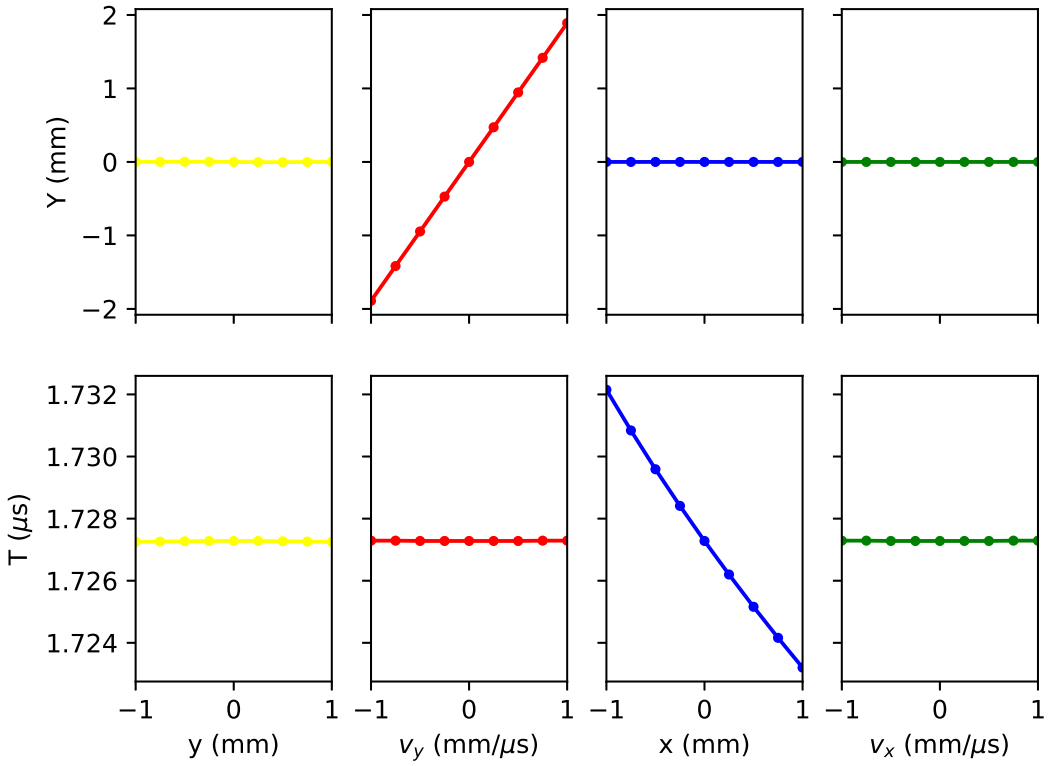

Figure 4: Y and T in function of y, v_y, x and v_x for $V_1 = 3000\,\mathrm{V}$ and $V_2 = 1995\,\mathrm{V}$.

dependency on v_y is so linear. We can see not null coefficients outside the diagonal, they are crossed terms of y and v_y with x, it is because the movement in the x axis breaks the linear behaviour of y and v_y, due to the shape of the complex electric field which the electrodes generate.

For the time of flight T we only observe a dependency on x at first order, it should be wrong, because in VMI mode it should depend on the velocity. Nevertheless we can see a brief curvature in the graphic, which we can observe in the unique not null element of the matrix $\partial^2 T/\partial x \partial v_x|_0$.

4.2 SMI mode

The results for the VMI mode are presented below, finally the best voltages were $V_1 = 3000\,\mathrm{V}$ and $V_2 = 2748\,\mathrm{V}$. In Figure 5 we can observe that for the coordinate Y there is only a strong dependency on y, while for T it is on x. The first approximation is good again. The coefficients for the first and the second order are presented below.

$$D^1_Y|_0 = \begin{pmatrix} -3.9697 \\ -0.0003 \\ 0 \\ 0 \end{pmatrix} \qquad D^2_Y|_0 = \begin{pmatrix} 0 & 0 & -0.1507 & 0 \\ 0 & 0 & 0.1823 & 0 \\ -0.1507 & 0.1823 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.6}$$

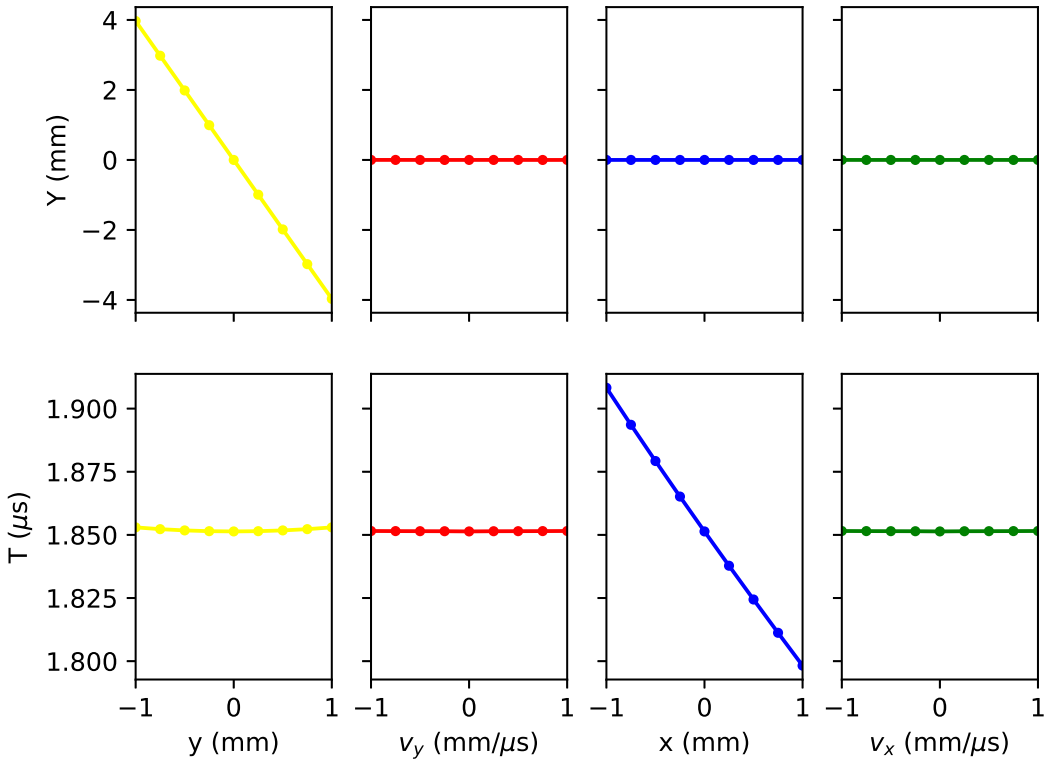

Figure 5: Y and T in function of y, v_y, x and v_x for $V_1 = 3000\,\mathrm{V}$ and $V_2 = 2748\,\mathrm{V}$.

$$D_T^1|_0 = \begin{pmatrix} 0 \\ 0 \\ -0.0549 \\ 0 \end{pmatrix} \qquad D_T^2|_0 = \begin{pmatrix} 0.0028 & 0.0008 & 0 & 0 \\ 0.0008 & 0.0002 & 0 & 0 \\ 0 & 0 & 0.0033 & 0 \\ 0 & 0 & 0 & 0.0002 \end{pmatrix} \tag{4.7}$$

We can observe that there is a really strong dependency on the Y coordinate, while there is not a real dependency on the rest of the variables, so, we have a good spatial map imaging mode. For T we observe a dependency on x, which is as we expected.

5 Velocity of the molecular beam

We determined the velocity of the molecular beam at the lab. At first, we determinated the position on the camera in the VMI mode in function of the TOF. Comparing the two graphics , we could find the masses. We made a least square regression (x^2 and m). As we had not a reference point (a good zero), it was neccesary to adjust the parameter C.

$$(x + C)^2 = k^2 m \tag{5.1}$$

where k is the magnification factor and m the mass. Plotting it 6, we obtained the best value $C = -265$. So, the obtained magnification factor is $k = 5.23$.

To find the velocity of the molecular beam, we use the following relation

$$x = kTOFv \tag{5.2}$$

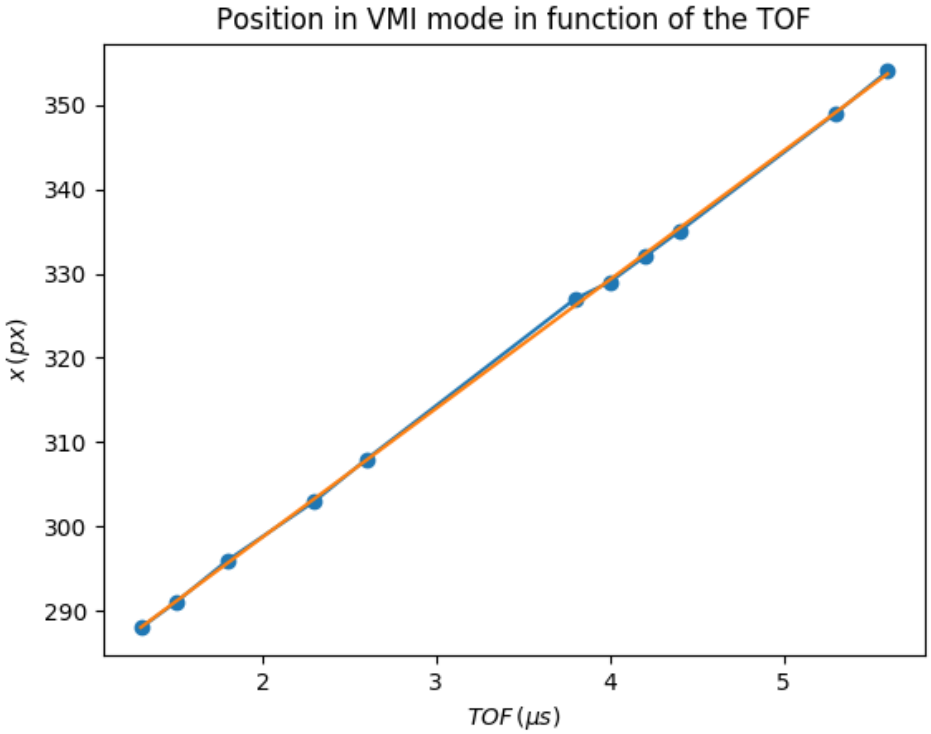

Figure 6: Results (blue) with its associated linear regression (yellow) for the position of the detector x in function of TOF.

where x is the position on the detector and v the velocity of the molecular beam. Taking the velocity of the molecular beam as constant, we can write that expression like this:

$$x = PTOF \tag{5.3}$$

where P is another constant. We could calculate P with our previous measurements. Finally, we obtained $P = 15.2675043\,\text{px/us}$ Knowing $8 \pm 2\,px = 1\,\text{mm}$ (VMI calibration 7).

$$P = 1.90843\,\text{mm/us} = 1908.43\,\text{m/s} \tag{5.4}$$

To obtain the velocity of the molecular beam we needed k, we could calculate it doing simulations with SIMION. We took an ion with mass $m = 254$ and the molecular beam was fixed in the position y=152mm and different initial velocities for the ions. In these simulations we worked in a VMI configuration with $V_1 = 3000\,\text{V}$ and $V_2 = 2000\,\text{V}$. We obtained $k = 1.00293$. Finally, we got the velocity of the molecular beam, $v = P/k$.

$$v = 1900 \pm 500\,\text{m/s} \tag{5.5}$$

We could also estimate the theorical value of the velocity v^*. Knowing that the tempeture was $T = 79\,\text{C}^\text{o}$ and $v = sqrt(5KT/m)$.

$$v^* = 1896\,\text{m/s} \tag{5.6}$$

So, our experimental value was close to the theorical estimation.

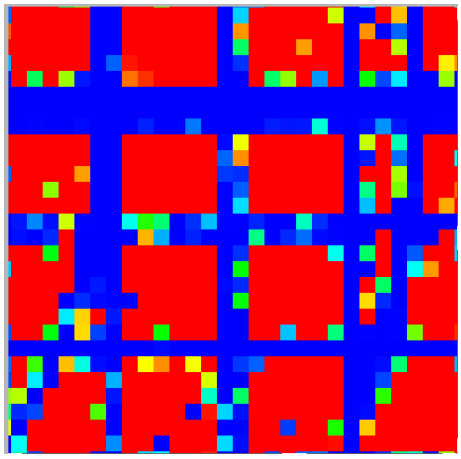

Figure 7: Picture of the VMI calibration

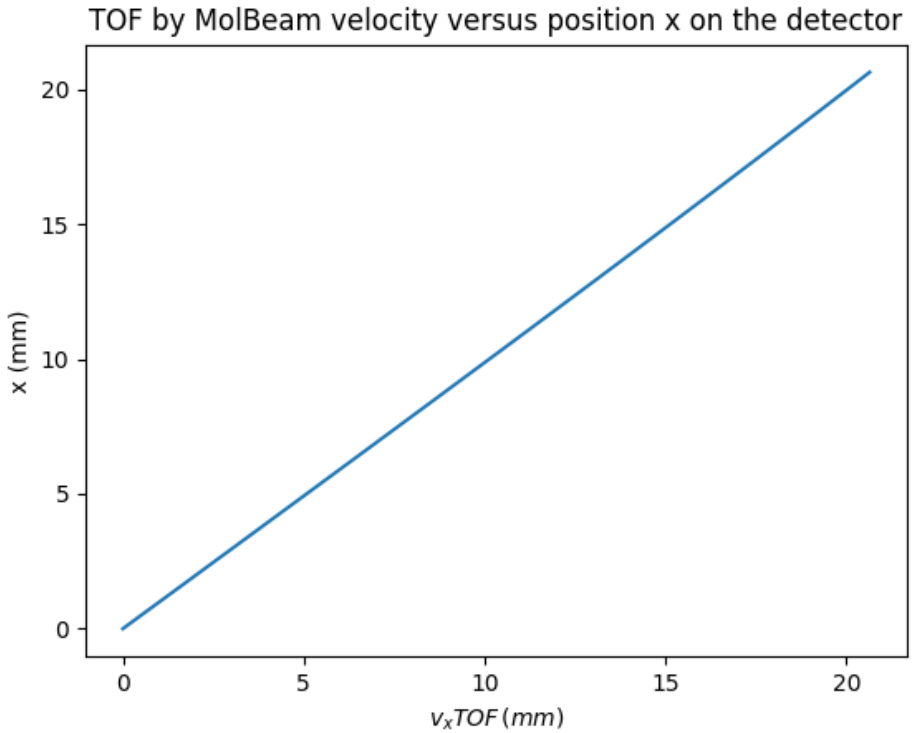

Figure 8: x in function of v by TOF.

References

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[4] Müller, N.(2016). Electron diffraction and controlled molecules.