Thick-Lens Velocity Map Imaging Spectrometer for High Energies

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An alternative method of measuring the energy of ionized electrons to the timeof-flight (TOF) spectroscopy method is velocity map imaging (VMI) spectroscopy. Using VMI spectroscopy, we can gather more information about the projected energy distribution of ionized electrons (i.e. angular distributions) as well as map them onto a two-dimensional plane.

The standard VMI model consists of a simple design of three electrodes (a repeller, extractor and a ground electrode) and a detector. An electrostatic lens that projects electrons onto the imaging detector can be formed with the application of appropriate voltages to the first two electrodes (the repeller and the extractor). The detector lies at a relatively long distance away from the three electrodes, a distance that is necessary in order to achieve high resolution. This detector is capable of measuring charged particles. However, because the detector is relatively far away from the electrodes, limits are imposed on the highest possible energies that can be detected. Typically, the standard VMI can measure electrons up to about 100 eV.

In recent years a new VMI has been designed and implemented in the JRM lab at Kansas State University. This design consists of many more electrodes and can potentially measure electrons with three-times the energy of highest measurable energies of the standard VMI (around 300 eV), with better resolution for all energies. The design has already been copied in Florida, Korea, and Australia. The purpose of this project was to characterize, through Simion simulations, the thick lens VMI, including finding the best possible set of voltages for the electrodes that produces the highest resolution for a range of electron energies. The results from these simulations were then compared to data from the standard VMI and experimental results. We found that the thick lens VMI results correlate closely with experimental data. Furthermore, this VMI achieves higher resolution than the standard VMI model up to a factor of 3.9.

Mapping Trajectories:

To observe the resulting distribution of electron energies in the thick lens VMI, we used an ion and electron optics simulator called Simion. Simion gave us the ability to reproduce the trajectories that the electrons would follow when released through an applied electric field.

In the set-up of our simulations, we specified a spot size of electrons that were released into the electric field from the interaction region. The spot consisted of 5 electrons: one in the middle and one to each of the four sides of it (shown in **Fig. [1]**). The diameter of our spot size was 2 mm, which over-estimates typical interaction regions by a factor of ~10. Many groups of electrons were defined where each group of electrons was assigned a specific energy within the appropriate range for the voltage on the repeller. This distribution of electron energies gave us the ability to see how the trajectories of each electron group were affected by the applied electric field.



Fig. [1]: Initial electron spot size used in our Simion simulations.

To set the electric field, a voltage drop was applied across the electrodes of the thick lens VMI. The thick lens VMI consists of 11 electrodes among which are the repeller, extractor, V_{focus} , and the ground electrode. A constant drop from the repeller to V_{focus} (generally set to 80%) of the repeller voltage and another constant drop between V_{focus} and ground creates an electrostatic lens. The percentage on V_{focus} , however, is tuned to show the best focusing ability of the electrostatic lens, depending on the voltage on the repeller. We found that the best percentage of V_{focus} when the repeller is set to -10 kV is 82% (-8200 kV).

The electrostatic lens is used to guide the trajectories of the electrons to a specific focal plane, in this case, the surface of the detector. A slice of the Simion view of the thick lens VMI set-up is shown in **Fig. [2]**. Equipotential lines can be seen in red. The shapes of the equipotential lines and the initial electron energy determine the path that the electrons will take. Each color of the electron group that hits the detector in **Fig. [2]** signifies a different initial electron energy range. Lower energies hit closer to the edge of the detector and higher energies hit close to the edge. A μ -shield is put in place on both sides of the VMI. The μ -shield has a potential of 0 V and prevents Earth or stray magnetic fields from penetrating the μ -metal surface and affecting the electric field lines.



Fig. [2]: (a) Diagram of the thick lens VMI. The repeller electrode is set to -10kV and V_{focus} is at 82% of the repeller (-8200kV). Electron energies range from 15eV to 360eV. (b) Electrons are projected in the same direction. Diameter of electron spot is 2mm. (c) Distance versus the voltage magnitude of the repeller, extractor, V_{focus}, ground, and detector, respectively.

Once we have the initial conditions defining the electron spot, we can simulate their trajectories. We set the "elevation angle" of the electrons to 90° to reflect typical laser experiments, as ionization tends to occur mainly along the laser polarization (see **Fig. [2], (b)**). In a real experiment, the electrons have a distribution of initial angles of velocity. However, 3-dimensional imaging can only be achieved after an inversion of the VMI images. This would require a lot more effort in the simulations, as we would have to follow the trajectories of a large ensemble of electrons to generate a full picture and then also apply an inversion technique. Instead, we choose only one angle to demonstrate the capabilities of the VMI.

Simion has many capabilities, one of which is recording the exact radius on the detector that the electrons hit. Knowing the resulting spot size of each electron-energy group allows us to analyze the data in several different ways. We can find the average resulting spot radius (Δy) of each group using the outer and innermost electron and compare it to the average resulting spot radius of the entire electron group (all of the electrons in the group). The numbers are almost identical- varying on the order of 10⁻¹, indicating that it is a good estimate. Knowing the resulting spot radius gives us the ability to find how precise the resolution of the thick-lens VMI is and how it compares to the standard VMI.

Calculating Resolution

If we were interested in finding the velocity with which an electron leaves its initial position we can simply use the basic kinematics equation (1). In this equation we signify v_v as the initial velocity that we are looking for, t as the time that it takes the

electron to hit the detector (assuming we know the time), and y as the distance that the electron moved from the middle of the detector in the "y" direction of our coordinate scale shown in **Fig. [1]** in the process of the flight.

$$v_y = \frac{y}{t} \tag{1}$$

To find the initial energy E_i of the electron, we use the kinetic energy equation (2).

$$E_{i} = \frac{1}{2}m(v_{x}^{2} + v_{y}^{2} + v_{z}^{2})$$
⁽²⁾

We fly the group of electrons in one direction, namely, the y direction. Therefore, $v_x = 0$ and $v_z = 0$, and we are left with the following equation:

$$E_i = \frac{1}{2} m v_y^2 \tag{3}$$

The next step is finding the percent energy error (or resolution), which we can calculate using the data we collect at the detector. The VMI technique uses an inversion procedure to reconstruct the z-momentum, which is much more complex to simulate. Therefore, distortions in the data due to the time of flight are not considered here, although they are expected to be small. Furthermore, the mass of the electron is known very precisely, leaving only the measured position on the detector as the main source of error to be considered in this work. To calculate the energy resolution, $\frac{\Delta E}{E}$, we determine the average resulting spot radius, Δy , at the detector. Then we apply error analysis to our energy function as shown in equation (4).

$$\Delta E_i = \frac{dE_i(y)}{dy} \Delta y \tag{4}$$

Taking the derivative of E with respect to y, we find that $\frac{dE_i(y)}{dy} = \frac{my}{t^2}$. Plugging this

back into equation (4), we see that $\Delta E_i = \frac{my}{t^2} \Delta y$. By dividing both sides by E_i , we arrive at:

$$\frac{\Delta E}{E} = 2\frac{\Delta y}{y} (\times 100), \tag{5}$$

which is the equation we use to determine the energy resolution

Analyzing Data

Knowing the resolution of the thick lens VMI spectrometer is important because it allows us to compare its resolution with the standard VMI spectrometer design. For the purposes of comparison, we modeled a standard VMI according to the dimensions used by Eppink and Parker [1] in 1997. The resolution abilities of the thick lens VMI model compared to the standard VMI model are shown by the resolution versus electron energy chart in **Fig.** [3]. We see that the thick lens VMI design produces significantly higher resolution than the standard VMI design by a factor of 3.9.



Fig. [3]: Resolution versus electron energy chart. The energies for these electrons vary from 15-360 eV. The voltage magnitudes of the repeller electrodes are 10 kV. For optimal resolution in each model, the extractor electrode of the standard VMI set to 9500kV and V_{focus} of the thick lens VMI set to 8200kV.

Higher voltages on the repeller were also tested to verify that we would get desirable results for higher electron energies. **Fig [4]** shows the resolution for the thick lens VMI model for a voltage of -30 kV on the repeller.



Fig. [4]: Resolution versus electron energy chart. The energies for these electrons vary from 50-1100 eV. The voltage magnitude of the repeller electrode is 30 kV. For optimal resolution, V_{focus} is set to 2800kV (80% of the repeller voltage).

According to Eppink and Parker [1], plotting the resulting ring radius found on the detector, \mathbb{R}^2 , against the kinetic energy of the electrons will produce a nearly linear plot, with some error from the linear behavior. We see this deviation clearly when we plot y^2 , denoted now as \mathbb{R}^2 , against E_i , shown by Fig. [5]. In this figure we also included a linear best-fit line which fits the equation y = 3.6483x + 24.918, where $\mathbb{R}^2 =$ 0.99898. Fig. [6] plots the residual, or difference in our original data points and the linear fit line points, so that we can see what kind of error we can expect. Fig. [6] clearly shows that the linear fit line works fairly well, but is not actually the best fit for our points.



Fig. [5]: R² versus electron energy chart with a linear fit line.



Fig. [6]: Residual versus electron energy showing the difference between the linearly fit line and original data points.

To find a better fitting equation to our points we tried several fits other than the linear fit. We found that the 2nd order polynomial fit, shown by **Fig. [7]**, is a much better fit. This is clearly shown when we compare the residual plots of the linear and polynomial fit cases, **Fig. [6]** and **Fig. [8]**, respectively. The polynomial equation is $y = -0.0013x^2 + 4.1255x - 1.407$ where $R^2 = 1$. The residual of the polynomial fit is almost 0, suggesting calibration methods should take this into account to minimize error.



Fig. [7]: R² versus electron energy chart with a 2nd order polynomial fit line. Compare to chart **Fig. [5]**, with linear fit line.



Fig. [8]: Residual versus electron energy showing the difference between the 2nd order polynomial fit line and original data points.

Comparing our Simion simulations to experimental data shows that the two agree very well. **Fig. [9]** shows the two curves on a resolution versus electron energy plot for our simulations and experimental data. Agreement of the first few points suggests that for

those electron energies (1.2 eV - 8.7 eV), the limiting factor in the resolution was coming from the spectrometer. The higher energies are almost flat, suggesting that the limiting factor for the resolution was the bandwidth of the laser pulses. These results show that our simulation is consistent with experimental data.



Fig. [9]: Resolution versus electron energy for our thick lens VMI simulations and experimental results. The voltage on the repeller was set to -799 V and the electron energies range from 1.2 eV to 19.9 eV.

Conclusion

The purpose of this project was to identify the capabilities of the thick lens VMI. Using simulations produced on Simion, we arrived at the conclusion that the thick lens VMI design produces results with higher resolution than the standard VMI design. After comparing our data with experimental data, we have concluded that our simulations for the thick lens VMI do, in fact, yield realistic results.

Works Cited

[1] A. T. J. B. Eppink and D. H. Parker, Velocity Map Imaging of Ions and Electrons Using Electrostatic Lenses: Application in Photoelectron and Photofragment Imaging of Molecular Oxygen, Rev. Sci. Instrum. 68, 3477 (1997).