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Method to compensate the dispersion of kinetic energy resolution in a velocity map imaging spectrometer

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Abstract

Here we present a novel method to improve the kinetic energy resolution of a velocity map imaging (VMI) spectrometer. The main modifications, compared to the original design of Eppink and Parker (1997 Rev. Sci. Instrum. 68 3477), are two additional grid electrodes. One of the electrodes is a grounded grid and the other is an arc-shaped grid with negative voltages (or positive voltages for an ions spectrometer). The arc-shaped electrode is axially symmetrical around the spectrometer axis. The field constructed by the two electrodes is to compensate the dispersion of the 'v'-shaped energy resolution. Simulations by SIMION and reconstructions by the basis set expansion Abel transform method show that the kinetic energy resolution can be improved drastically by our new method. Furthermore, the accuracy in the determination of the kinetic energy of ion/electrons remains unchanged with respect to the original design.

Keywords: velocity map imaging spectrometer, kinetic energy resolution, dispersion-compensated velocity map imaging

(Some figures may appear in colour only in the online journal)
of the particles is perpendicular to the flight tube. With the electrostatic lens, ions/electrons with the same initial KE are focused onto the same spot on the detector plane (green line). This ability of the electrostatic lens leads to a strong deblurring of the recorded images. However, in a typical VMI, the focal plane (yellow line) of particles with different initial KE does not overlap with the detector plane. This is because the focal plane is not perpendicular to the flight tube. Due to this effect, the size of the spots on the detector plane is not the minimum size, except on the crossing point of the detector plane and focal plane. The spot is formed by the hitting of the particles with the same KE. As shown in the right panel of figure 1(a), the relationship between the size of the spots and the initial KE is a ‘v’-shaped curve. The KE resolution is given by:

$$\Delta E/E = 2 \times (\Delta r/r).$$

where $\Delta r$ is the size of the spots and $r$ is the displacement with respect to the center of the detector. Hence the relationship between the resolution and the initial KE is also a ‘v’-shaped curve, which can be considered as a dispersion.

Since the VMI technique was introduced, improved designs have been reported [16–18]. However, no method has been available for compensating the KE dispersion. In this article, a novel design of VMI, which is called ‘dispersion-compensated VMI (DVMI)’, is introduced and its performance in compensating the resolution dispersion is investigated thoroughly. Details of the DVMI are discussed in section 2. In section 3, we discuss the performance of the DVMI by comparing with the typical VMI. In section 4, we conclude our work on improving the energy resolution of VMI, with the numerical results.

2. Overview of the dispersion-compensated VMI

Figure 1(b) shows a sketch of the DVMI. In comparison to the typical design, the main modification is an additional deflection field. The deflection field is constructed by a grounded electrode and a deflection electrode. The field makes the flight trajectories of the particles bend to the tube wall. Deflection of the trajectories by an angle $\theta$ (in figure 1(b)) is a decreasing function of the initial KE. This bending effect makes the electrons with low KE focus in advance along the tube axis, therefore the focus plane can overlap with the detector plane. As a result, $r$ is enlarged and $\Delta r$ is reduced. According to equation (1), it can be expected that the dispersion will be well compensated, and the energy resolution will be improved drastically.

In the original VMI design of Eppink and Parker, all of the electrodes are plates with holes. However, the recent introduction of grids makes the VMI spectrometers present some new advantages [18, 19]. In our work, we apply two grids to generate the deflection field and a grid grounded electrode to separate the free drift region from the acceleration region. The transmissions of each grid is 90%, and the transmission of the total grids can be higher than 70%. The transmission of 70% is acceptable, especially in the experiments with a high power pump laser. For the curved grid in figure 2(b), similar conical grids can be found in [20–22].
3. Simulation results and comparison

To demonstrate the performance of DVMI, we use SIMION to simulate the imaging process. Detailed electrode setups of the two designs are given in figure 2. In VMI, the tube length is related to the maximum kinetic energy release. Generally the detection of particles with large kinetic energy releases needs a short tube length. In our work, the tube length of the typical VMI and DVMI is 120 mm, which is typical for experiments with high kinetic energy release [23]. For the typical VMI, voltage on repeller (Vr) = −5000 V and voltage on extractor (Ve) = −4285 V. For the DVMI, the voltage on repeller (Vr) = −2500 V, voltage on extractor (Ve) = −1790 V and voltage on deflector (Vd) = −190 V. The grid electrode G in the DVMI is applied to reduce the impact of the acceleration field to the drift area. For comparison, in the DVMI the distances from the electrodes E, G and the detector to the electrode R are identical to that of the typical VMI.

The interaction region of the laser and the molecular beam is located in the middle of the electrodes R and E. The laser is linearly polarized along the z-axis (in figure 2) and propagates along the y-axis. The size of the interaction region along the y-axis is 1.0 mm, and the size along the x-axis, which is the minimum beam waist of the laser, is 20.0 μm. The initial KE ranges from 10 eV to 100 eV with an interval of 5 eV. In above threshold ionization (ATI) experiments, the kinetic energy releases of the photoelectrons can reach to 100 eV [24].

3.1. Results from 2D initial velocity distribution

Firstly, we assume that the initial velocity distributes in the y–z plane (in figure 2) uniformly. With this kind of distribution, nearly no noise is produced. Therefore, without reconstruction, we can calculate the resolution with the positions of impact of the particles recorded on the detector plane. A comparison of the resolution between the two VMI designs is shown in figure 3. We find that the resolution of the DVMI (red line) almost remains the same value, which is lower than the minimum value of that of the typical VMI (blue line). Additionally, the worst resolution of 0.4% of the DVMI is also quite remarkable, comparing with the value of 2.7% of the typical VMI.

3.2. Results from 3D initial velocity distribution

Next, a 3D distribution is adopted as the initial velocity distribution in the simulation and the angular distribution was assumed to be isotropic. Flight trajectories of 1.0 × 10^6 photoelectrons are simulated by SIMION. Then an image containing noise can be obtained on the detector. The noise is produced by photoelectrons whose velocity vector is unparallel to the y–z plane. To get the initial 3D velocity distribution, a basis set expansion (BASEX) Abel transform method [14] is applied for image reconstruction. With the above simulations, we have mimicked an imaging experiment of photoelectrons using a VMI spectrometer and the initial KE distribution of the photoelectrons can be reconstructed by the simulated VMI spectrometer.

Figures 4(a) and (b) show the raw images recorded by the detector. Using the BASEX method, the 3D distributions can...
be retrieved from the 2D raw images. The 2D cuts of the 3D distributions are shown in figures 4(c) and (d), from which one can clearly see the sharp rings. The different rings are formed by electrons with different KE. Figure 5 shows the relationship between the radius of the rings and the square root of KE. One can find that the relationships in the typical VMI and the DVMI are all linear. The fit line of the relationship of the DVMI do not go through the origin, which has an intercept of $-0.55$. The intercept will produce a measurement error of $0.3\%$. The intercept is proportional to the square root of the maximum KE. For the maximum KE of 10 eV, the error will be only 0.03 eV. With figures 4(c, d) and 5, we plot the KE distribution in figure 6. Figure 6(a) shows a good agreement between the initial KE distribution (green) and the KE distribution retrieved by the DVMI (red). In figures 6(b)–(d), we compare the KE distribution retrieved by the typical VMI

Figure 4. Images recorded by the detector and 2D cuts of the image reconstructed by the BASEX method. (a) Image recorded by the detector of the typical VMI. (b) Image recorded by the detector of the dispersion-compensated VMI. (c) 2D cut of the reconstructed image of the typical VMI. (d) 2D cut of the reconstructed image of the dispersion-compensated VMI.

Figure 5. The relationship between the radius and the square root of KE. The blue line is the data from the typical VMI and the red line is from the dispersion-compensated VMI. The two green lines are fit lines.
and DVMI at 10 eV, 40 eV and 95 eV respectively. It can be found that the widths of the peaks retrieved by the DVMI are narrower than that retrieved by the typical VMI. $\Delta r$ is then obtained as the full width at half maximum (FWHM) of the KE distribution. The differences of $\Delta r$ between VMI and DVMI are seemingly slight. It should be noted that the resolution is defined by $2\Delta r/r$. Reducing $\Delta r$ is only one aspect contributing to the improvement of resolution. In DVMI, $r$ is enlarged slightly by the deflection field, which also contributes to the improvement of the resolution. By equation 1, the energy resolution can be calculated. Figure 7 shows a comparison of the resolution between the typical VMI and the DVMI after reconstruction. The energy resolution of the DVMI is obviously better than that of the typical VMI. Comparing with figure 3, in figure 7 the improvement of the resolution at the condition of the 3D initial distribution turns out to be smaller. This is because the DVMI can not compensate well the dispersion from the photoelectrons whose initial velocity vector is unparallel to the $y$–$z$ plane. Even though the compensating mechanism is affected by this issue, the worst resolution of the DVMI is still only half of that of the typical VMI. It indicates that, for 3D initial velocity distribution, the DVMI also perform well on improving the KE resolution.

4. Discussions and conclusions

Nowadays the use of many electrodes to create a smooth, slow extraction field in combination with a fast gated detector to detect only the center slice of an image has become a popular approach to detect the KE distribution of photoelectrons/ions. The method of using many electrodes to create a smooth field is useful to improve the KE resolution. But the resolution dispersion effects still exist. It is the electronic lens that produces the dispersion effect. This imaging approach also needs an electronic lens to spatially focus the electrons/ions with the same KE onto a target point. To remove the dispersion, the dispersion needs to be compensated.

For ion experiments the Micro-Channel Plate (MCP) needs to be polarised at high negative values to improve efficiency. Also, for threshold electron detection where the extraction field is kept very low [25–27], the MCP needs to be positively polarised at a few hundred volts to maintain efficiency. Then, we need to consider how to remove the impact of the high voltage of the MCP on the deflecting field. Generally, a suit of MCP is made up of two pieces of MCP plates. In our work, we grounded the first MCP plate and applied the high voltage on the second MCP plate. Therefore, the front of the first MCP plate plays the role of removing the impact of the high voltage of the MCP on the deflecting field.

In this work, we have presented a novel design of a VMI spectrometer called the ‘dispersion-compensated VMI’. The benefit of the DVMI is that it compensates the dispersion of the ‘v’-shaped energy resolution in the typical VMI successfully and obviously improves the resolution. We realize this idea by making the inclined focal plane perpendicular to the flight tube. Electron trajectory simulation by SIMION shows that the focal plane in the DVMI is perpendicular to the tube and well superposed with the detector plane. Simulation of the imaging process has demonstrated the remarkable performance of the DVMI in improving the VMI resolution. With the application of the dispersion-compensated method, the VMI spectrometer will be a more powerful tool in chemical physics.

Acknowledgments

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