Molecular Beam Velocities

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March 23, 2014

Summary

In this document, the results obtained from a series of molecular-beam velocity-map imaging experiments are described. In these experiments gas mixtures either Ar, He, and CO in various proportions and flow rates were subjected to a coarse temperature range ($\sim 25 - 1250\,^{\circ}\mathrm{C}$) using a μ-tubular flow tube reactor with an inner diameter (ID) of either 0.66 or 1.0 mm. The nacent molecular beam was ionized by VUV radiation and imaged by a Roentdek delay-line imaging apparatus. The resulting data was processed using the openCV 'computer vision' libraries implemented under Python.

1 Experimental Description

A skimmed molecular beam emanating from the nozzle orrifice is probed by vacuum-ultraviolet (VUV) light. Nacent ions are measured by velocity-map imaging using a delay line imaging apparatus. A more thorough description available upon request.

2 Data Analysis

The data are organised according to nozzle diameter > molecular system > gas mixture ratio. For example, Ar in He using the 600 μm nozzle can be found in `600` > `Ar` > `2pc`. In each of these directories can be found the results of the data analysis.

The data analysis procedure can be summarized accordingly:

1. centroid images to determine molecular beam and background component center positions
2. fit a sum of two gaussian functions through the centroids
3. determine a per pixel distance for the data based on the known photodissociation of O_2.

A more thorough description of this procedure follows.

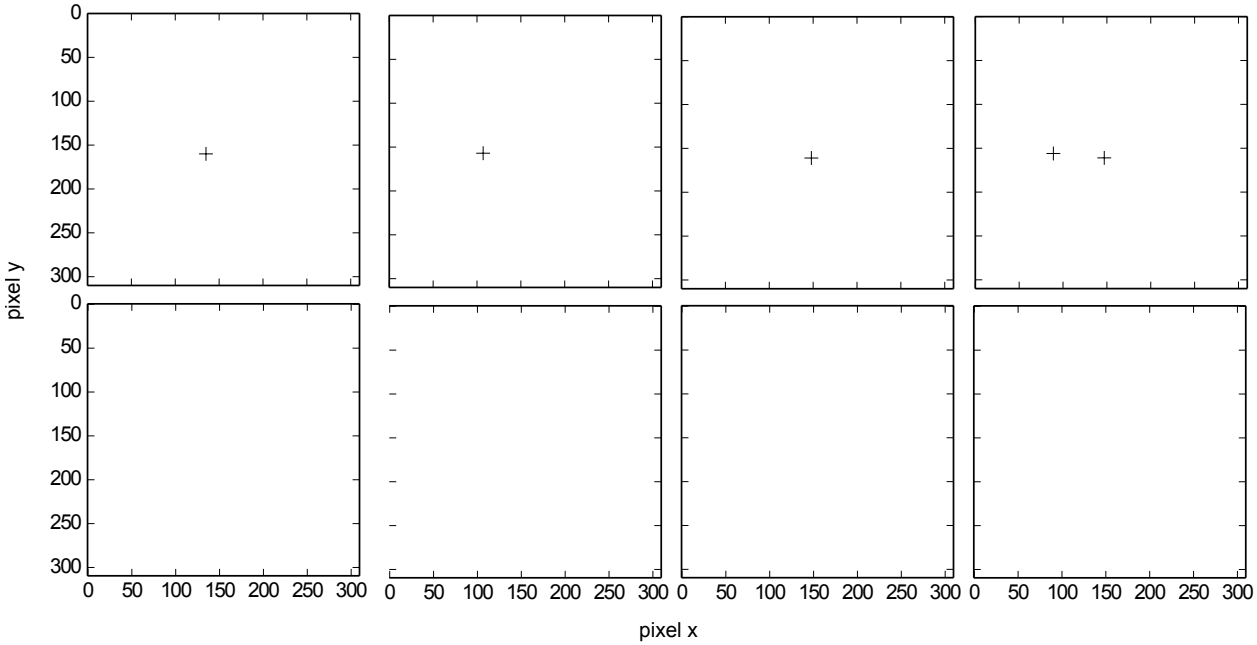

Figure 1: The images of a room temperature molecular beam image of 2 % CO in He and the effects of masking in centroiding (A-C) compared to a hot molecular beam image (D). An unmasked image results in the centroids and contours seen in A1 and A2, respectively. The introduction of masking allows for the centroiding and contour analysis of both molecular beam (B1, B2, respectively) and the background (C1, C2, respectively). D1 and D2 show the centroids and contours found where the background and molecular beam components are well separated in space and requires no mask intervention.

2.1 Centroiding and Distribution Fitting

2.1.1 Centroiding and Masking

Centroiding is a process that determines the center of a particular region of an image. This can be done efficiently by use of centroiding software. In this work, centroiding is achieved by use of the OpenCV2 Computer Vision libraries implemented with the Python programming language. Briefly, the implemented script normalizes the image data and creates a contour representation of it based on a user supplied threshold. From these contours, centroiding can be performed.

An extra step is required for room-temperature (RT) images including O_2 or any case where molecular beam and background components overlap. In these cases image masking is performed before centroiding. This step requires subjective intervention since the masks are manually set. This difference is illustrated in fig. 1 which contains an example of both hot and RT images after contour and centroiding treatments.

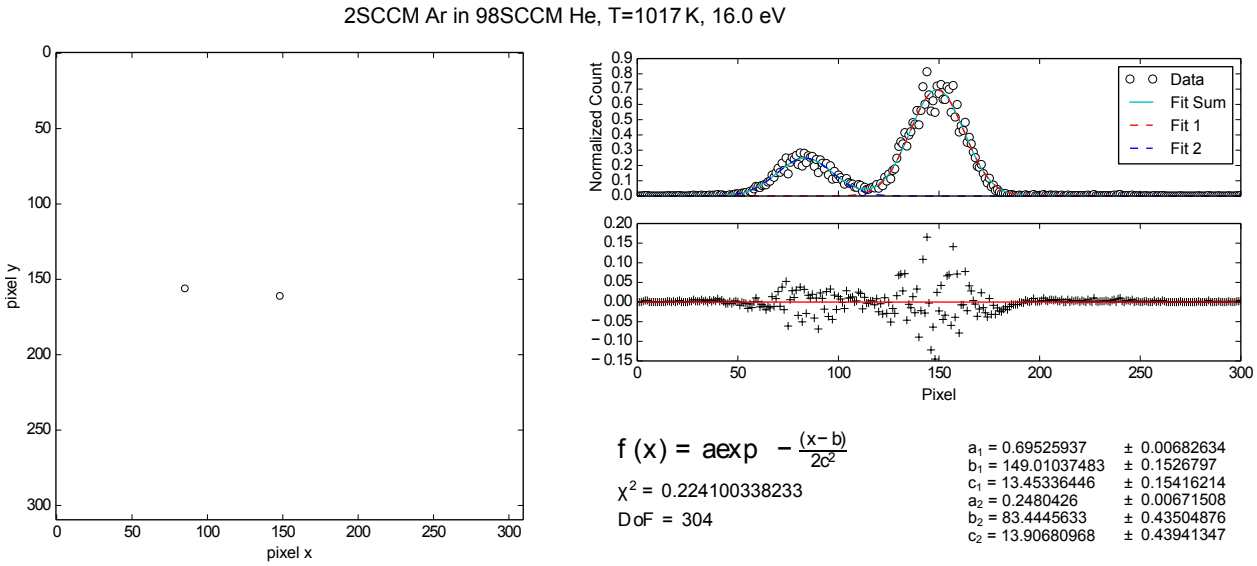

Figure 2: The data under the line mapped through the centroids (LEFT). A sum of two gaussians is then fit to the extracted line to determine the velocity distribution in that axis. (RIGHT)

2.1.2 Fitting the line through centroids

Once the centers of both the background and the molecular beam are found by centroiding, we can fit the two components to a function represented by the sum of two gaussian functions to determine the uncertainty of this position. This is achieved by a separate script which maps the line between the component centroid pixel coordinates and fits a gaussian to each component. The outcomes of this procedure are illustrated in fig. 2.

This fit gives us the distance in pixels between the background and molecular beam components. Now, a conversion from pixels to meters is required. This is achieved by imaging of a system with a known energy. In our case, we use the photodissociation of oxygen.

2.2 Determining the pixel/distance relationship

To determine the absolute distance represented by one pixel, we turn to the photodissociation of O_2. O_2 ionizes above 20.0 eV to form O^+ and O^-:

$$O_2 \xrightarrow{>\sim 20.0\,eV} O^+ + O^-$$

The O^+ forms with a constant 0.8 eV kinetic energy, E_k, component. From this we can determine the O^+ velocity, v, using:

$$E_k = \frac{1}{2}mv^2 \rightarrow v = \sqrt{\frac{2E_k}{m}}$$

Calculating these terms for O^+, first E_k:

$$\begin{aligned} E_k &= 0.8 \cdot \text{eV} \times 1.60217657 \times 10^{-19} \\ &= 1.3 \times 10^{-19} \cdot \mathbf{kg} \cdot \mathbf{m^2} \cdot \mathbf{s^{-2}} \end{aligned}$$

and m:

$$\begin{aligned} m &= \frac{15.9994 \cdot \mathbf{g} \cdot \mathbf{mol^{-1}}}{6.022 \times 10^{23} \cdot \mathbf{mol^{-1}}} \\ &= 2.7 \times 10^{-23} \cdot \mathbf{g} \\ &= 2.7 \times 10^{-26} \cdot \mathbf{kg} \end{aligned}$$

now v:

$$\begin{aligned} v &= \sqrt{\frac{2 \times 1.3 \times 10^{-19} \cdot \mathbf{kg} \cdot \mathbf{m^2} \cdot \mathbf{s^{-2}}}{2.7 \times 10^{-26} \cdot \mathbf{kg}}} \\ &= 3106.2 \cdot \mathbf{m} \cdot \mathbf{s^{-1}} \end{aligned}$$

This velocity must now be related to a distance according to:

$$d = vt$$

For O^+, we have our velocity, v. t refers here to the flight-time of O^+. Due to difficulties in obtaining reliable times-of-flight (TOF) with the spectrometer in imaging mode, TOF were calculated using the ion simulation software Simion using the spectrometer voltage settings and dimensions as inputs. The calculated times are sensible with respect to the broad flight-time distribution we see in the data. For O^+ this flight time is $4.76 \times 10^{-6} \cdot \mathbf{s}$. So our distance is:

$$\begin{aligned} d &= 3106.2 \cdot \mathbf{m} \cdot \mathbf{s^{-1}} \times 4.76 \times 10^{-6} \cdot \mathbf{s} \\ &= 1.48 \times 10^{-2} \cdot \mathbf{m} \end{aligned}$$

Finally we can determine what is the distance per pixel. We do this by dividing the distance traveled by the O^+ by the number of pixels between the centers of the O_2 molecular beam component and the O^+ photodissociation component. fig. 3 shows the line of data used for fitting. With a travel distance of 73 pixels, we find a per pixel distance of:

$$\begin{aligned} \text{Per pixel d} &= \frac{1.48 \times 10^{-2} \cdot \mathbf{m}}{73} \\ &= 2.01 \times 10^{-4} \cdot \mathbf{m} \end{aligned}$$

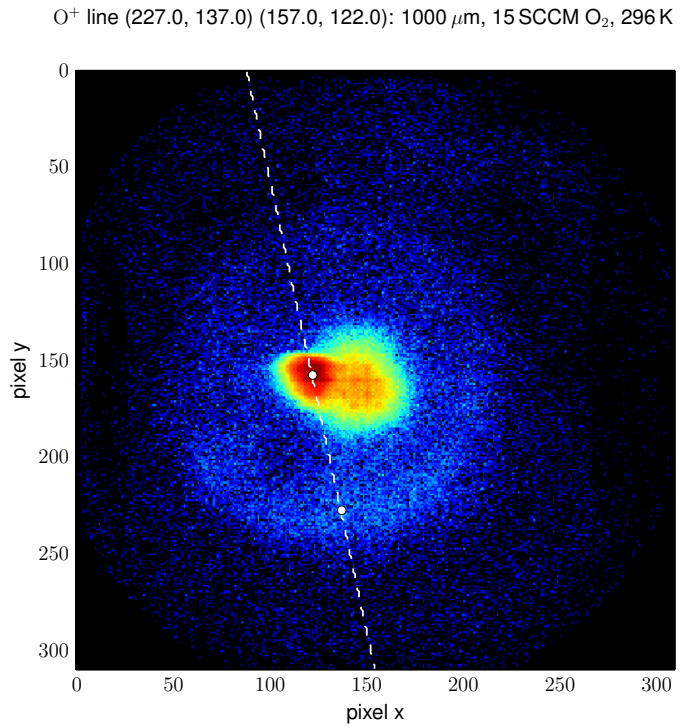

Figure 3: The slice used for determining the O^+ to O_2 distance in pixels.

The accompanying Excel spreadsheet, "`VelocityWorkup.xlsx`" demonstrates these step-by-step calculations. Finally this per pixel distance factor is then applied to the thermal reactor data for which velocities are calculated according to:

$$v = \frac{d}{t}$$

Applying this pixel to distance relationship to the data allows us to determine the velocities at each temperature to produce temperature versus velocity plots such as fig. 4

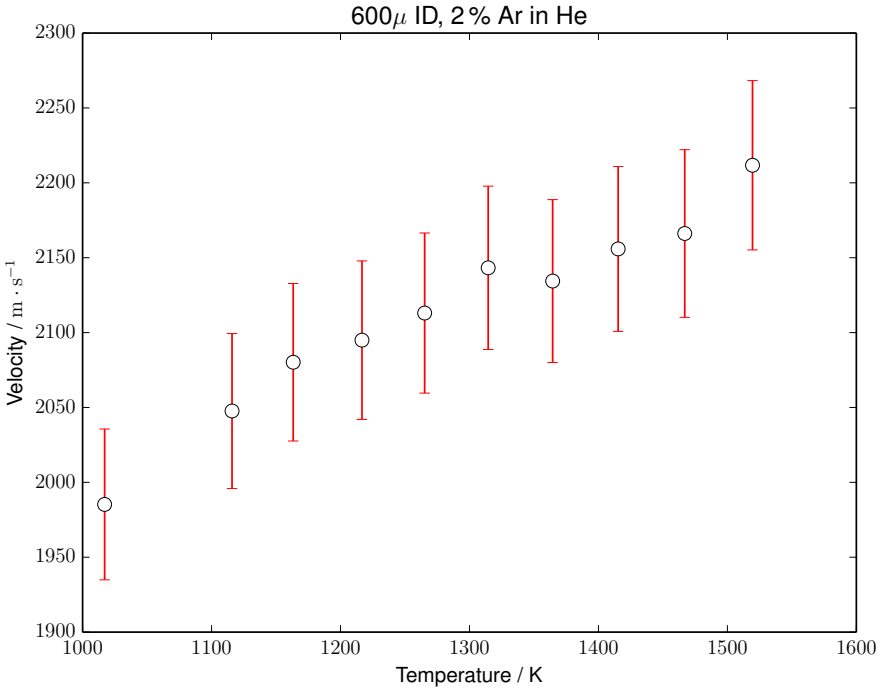

Figure 4: The velocities of a molecular beam containing 2 % Ar in He at varying temperatures.