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Momentum imaging of the phofragments from fullerenes.

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[Introduction]

We are developing a mass-selected momentum imaging spectrometer to observe the momentum distributions of the scattered fragments produced from dissociative ionization of gaseous C_{60} at the BL2B in the UVSOR synchrotron radiation facility. We have adopted the Eppink-Parker type three element velocity focusing lens system [1] (Repeller, Extractor, and Tube electrodes) to achieve the high kinetic energy (K.E) resolution on the photofragment images. It is known that there are two possible mechanisms on the fragmentation processes [2, 3], namely the sequential ejection of C_2 units

$$C_{60}{}^{z+} \rightarrow C_{58}{}^{z+} + C_2,\ C_{58}{}^{z+} \rightarrow C_{56}{}^{z+} + C_2,\ \ldots\ldots,$$
$$C_{60\text{-}2n+2}{}^{z+} \rightarrow C_{60\text{-}2n}{}^{z+} + C_2\ (n \geq 1,\ z \geq 1) \text{ -------- (i)}$$

and the fission of $C_{60}{}^{z+}$ to directly produce a final fragment

$$C_{60}{}^{z+} \rightarrow C_{60\text{-}2n}{}^{z+} + C_{2n} \text{ -------- (ii)}$$

Several groups tried to distinguish the two mechanisms by measuring the total average kinetic energy (K.E) release in the decomposition of C_{60} into its fragments [4, 5]. But they could not conclude because the two mechanisms give almost the same total average kinetic energy release. Before experiment we are verifying by means of computer simulation whether or not these two mechanisms give different shapes of image, or different momentum distributions of $C_{56}{}^{+}$. We also made the data analysis programs suitable for the photofragment imaging and examined the performance of the program using artificial inputs.

[Simulation method]

In the momentum imaging technique the 3D momentum distributions of fullerene photofragment ions are projected on the 2D position sensitive detector (PSD). We performed Monte Carlo simulation to generate the momentum images with conditions expected in our experiment as: TOF (Time of Flight), 50 μs; the number of ions hitting at the surface of PSD, 8×10^5; Temperature of the C_{60} molecular beam, 0 K and 273 K. The kinetic energy release for C_2 and C_4 ejection is assumed to take a constant value of 0.4 eV, to a first approximation. Angles of ejection are selected randomly under the condition of isotropic angular distributions.

[Simulation result and Discussion]

The simulated images of the fragment ion $C_{56}{}^{+}$ from C_{60} through mechanisms (i) and (ii) are depicted in Fig. 1. From the image result it is clear that at the temperature of 0 K the two mechanisms are well distinguished, but with increasing beam temperature two mechanisms are hardly distinguishable. The experimental image of $C_{56}{}^{+}$ is a convolution of the momentum distribution of parent C_{60} in the beam and that of $C_{56}{}^{+}$ produced by the reaction. To extract the scattering distributions of $C_{56}{}^{+}$ image from the convolved experimental image we have two plans namely: data analysis by deconvolution and the improvement of the experimental setup.

Deconvolution is a process which is used to reverse the effect of convolution for obtaining the image data. We are performing the deconvolution procedures of images by using the 2D Fast Fourier Transform (FFT) and Inverse Fast Fourier Transform (IFFT). In the real experimental observation usually some noise is added to the convolved image. We need to check the trends of noise during deconvolution procedure because, deconvolution is very much noise-sensitive in the image data transformation. So, we have generated the 2D sample image which is a convolution of two circles with their radii 31 (Fig.2a) and 15 (Fig.2b) pixels, respectively, in 128×128 data array. Then randomly scattered dots are added to simulate the noise. The ratio of the noise is 0.25% of the total intensity of the sample image. The convolved image is shown in Fig.2c. The blurred width of the image is 30 pixels which correspond to the diameter of the circle in Fig.2b.

We performed deconvolution of Fig.2c using Fig.2b and obtained Fig.2d. In Fig.2d the circle with the same diameter and line width as Fig.2a can be seen. This deconvolution process therefore, successfully recovered the original image; however, a large amount of noise is also observed in this image. The momentum distribution can be affected by the noise if we apply this procedure to the experimental images. Low pass filter will improve the signal to noise (S/N) ratio. More essentially, the experimental effort to decrease the C_{60} beam temperature will allow us to minimize the effect of this unstable “inverse problem”, and to obtain more directly the scattering distribution of photofragments. We are planning to design new fullerene beam source utilizing co-expansion with rare gases or collision cell filled with rare gases.

[Reference]

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[2] K. Mitsuke et al. AIP Conf. Proc. 811 (2006) 161. [3] B. P. Kafle, et al. AIP Conf. Proc. **879**, 1809 (2007). [4] H. Gaber et al. Z. Phys. D **24**, 302 (1992). [5] D. Muigg et al. J. Chem. Phys. **108**, 963 (1998).

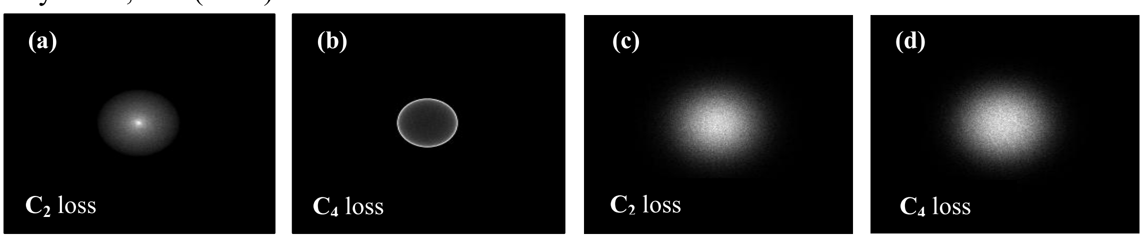

Fig. 1: Simulated 2D projections of the 3D scattering distributions of C_{56}^+ fragments (image size: 40 × 40 mm). (**a**) and (**c**), sequential ejection of C_2 units; (**b**) and (**d**), Fission of C_{60}^+. The beam temperature is 0 K for (**a**) and (**b**) and 273 K for (**c**) and (**d**).

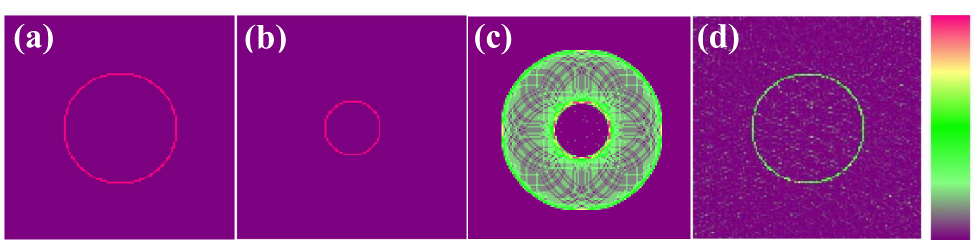

Fig.-2: (**a**)–(**b**) 2D original images (circles with radii 31 and 15 pixels, respectively);
(**c**) Noise-mixed convolved image with blurred width of 30 pixels and
(**d**) Recovered Image (same as (**a**) except noise blurred);
Image size: 128 ×128 pixels.