



	Experiment title: Structure of Nitrogen- and Sulphur- doped Carbon dots through Pair Distribution Function Analysis	Experiment number: SC 4353
Beamline: ID22	Date of experiment: from: 9/10/2016 to: 10/10/2016	Date of report: 27/02/20
Shifts: 3	Local contact(s): Mauro Coduri	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

* Dr. Fabrizio Messina Università di Palermo, Dipartimento di Fisica e Chimica, Via Archirafi 36, IT - 90123 PALERMO

* Miss Alice Sciortino Università di Palermo, Dipartimento di Fisica e Chimica, Via Archirafi 36, IT - 90123 PALERMO

* Dr. Luisa Sciortino Università di Palermo, Dipartimento di Fisica e Chimica, Via Archirafi 36, IT - 90123 PALERMO

Report:

Carbon Dots (CDs) are a new class of nanomaterials which has attracted a remarkable interest in the last ten years. They are carbonaceous nanoparticles exhibiting a broad intense emission with marked excitation-wavelength dependence and excellent biocompatibility. As a consequence, a wide range of possible applications has been proposed for CDs, such as imaging agents, nanosensors sensitive to metal ions, lasing and many more. In the world of CDs, N-doped dots stand out for their high fluorescence

Quantum Yield (QY), very outstanding for applications. Due to the poorly crystalline structure and to nanometric size, the structure of CDs has been quite difficult to study and remains unknown in most cases, hindering a deep understanding of the fundamental nature and properties of these nanomaterials. The proposed experiment aims to study the structure of CDs and to reveal the effect of nitrogen doping on CDs by the analysis of the Pair Distribution Function (PDF).

We carried out our experiment using $\lambda=0.190758 \text{ \AA}$ (65 keV) and the detector 2D(41 cm*41 cm, 100 μm *100 μm pixel) at 38-38.5 cm to the capillary. The transmitted beam was centered in the top right corner of the detector to increase as much as possible the Q range. For each image, the integration time was set at 5 s, and the background was subtracted for each image. The size of the collimated beam was 500 μm .

We collected the diffraction pattern of two different series of samples with different content of nitrogen. The series named “acu074” contains a nominal atomic ratio N/C equal to 0.74 and the series named “acu014” contains a nominal atomic ratio N/C equal to 0.14. Both series were measured as pristine and after an *ex-situ* thermal treatment in air for 1 hour at 300°C and 400°C. All samples are powders and are measured sealed in a borosilicate capillaries. The $G(r)$ functions were extracted using the software PdfgetX3. In figure 1 we report the $G(r)$ for the acu074 series pristine and after thermal treatment in air at 300°C and at 400°C.

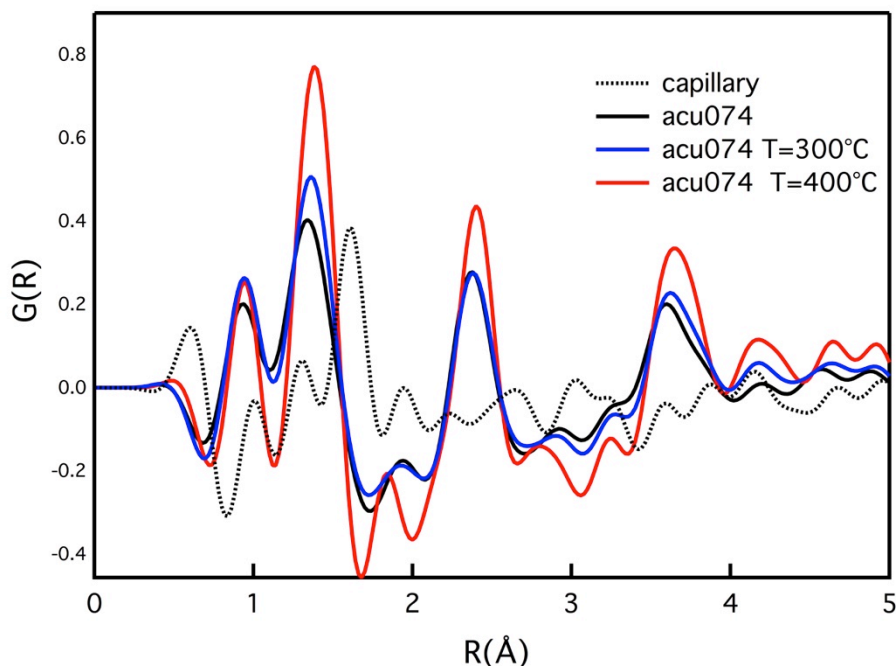


Figure 1. $G(r)$ of the series acu074 pristine (black line) and after thermal treatment in air at 300°C (blue line) and at 400°C (red line).

In figure 2, we report two different data for the pristine samples of both series to underline the difference with different content of nitrogen.

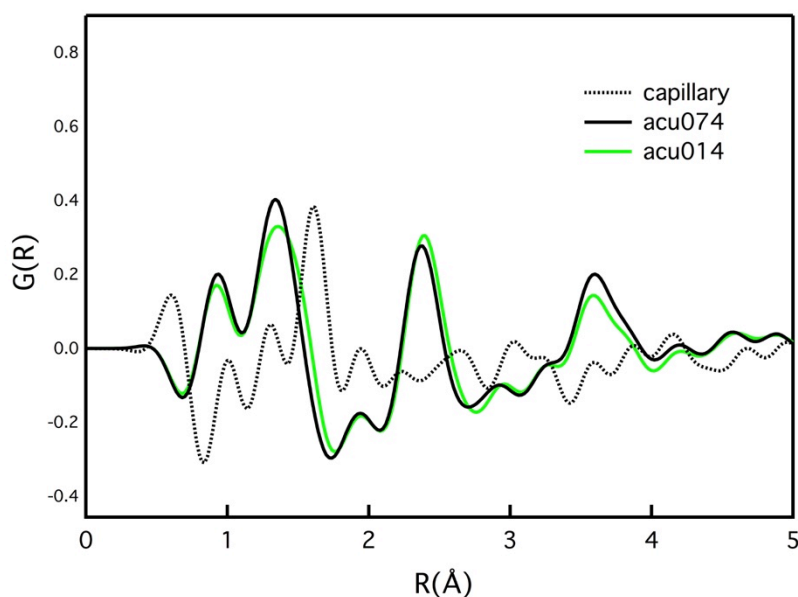


Figure 2. $G(r)$ of the series acu074 pristine (black line) and of the acu014 pristine (green line).