Benchmark Data to Publish on the International Fluid Properties Simulation Challenge (IFPSC) Website (http://fluidproperties.org/)
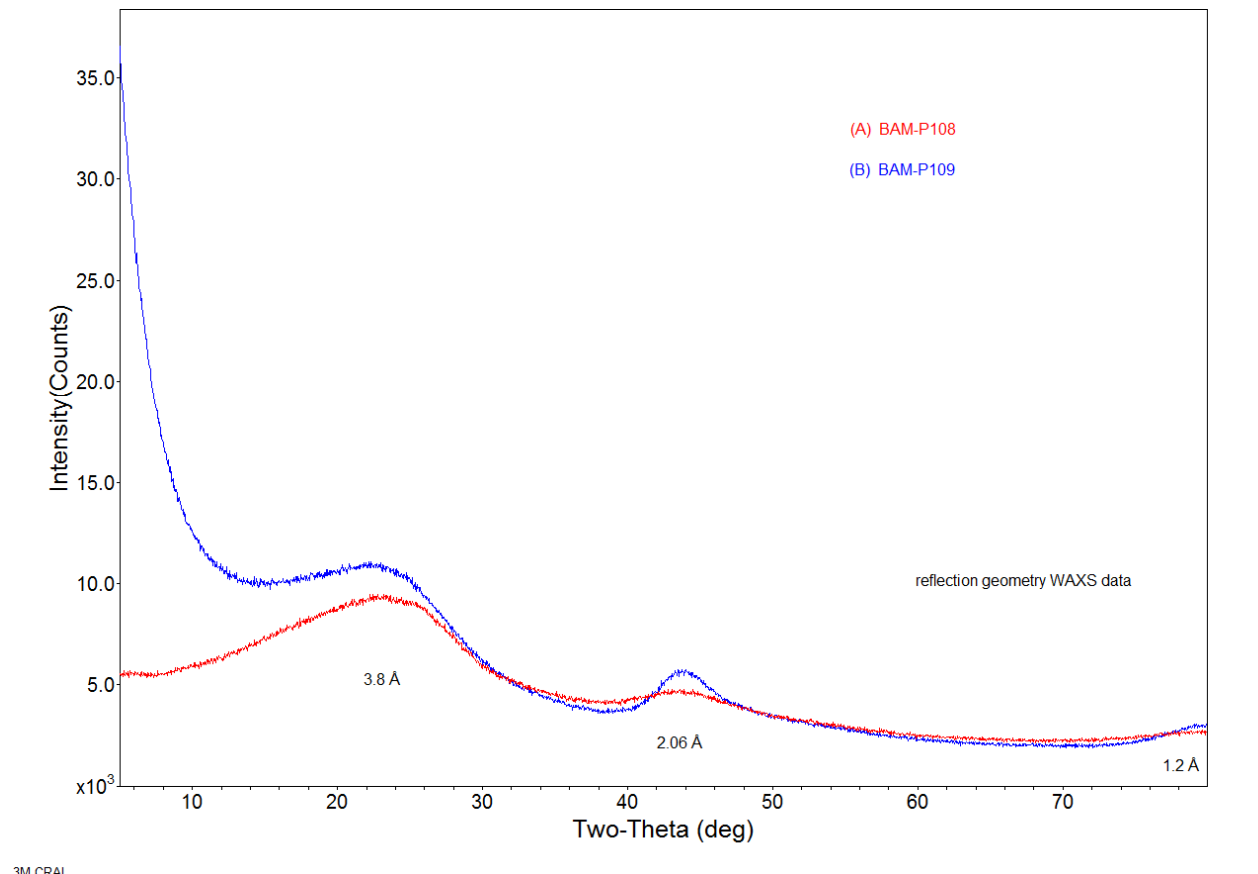
- This data was measured by 3M for the 8th International Fluid Properties Simulation Challenge which focuses on predicting adsorption of perfluorohexane onto the certified reference material BAM P109 standard activated carbon.
  - For info on BAM P109 see: http://www.rm-certificates.bam.de/de/rm-certificates_media/rm_cert_porous_materials/bam_p109e.pdf

- X-ray diffraction, X-ray photoelectron spectroscopy, and elemental analysis have been carried out on the BAM P109 activated carbon. Some data for comparison is also posted for the BAM P108 activated carbon.

Summary of Studies and Slides

* Slides 2-7: X-ray Diffraction and Tomography Studies

* Slides 8-10: X-ray Photoelectron Spectroscopy (XPS/ESCA)

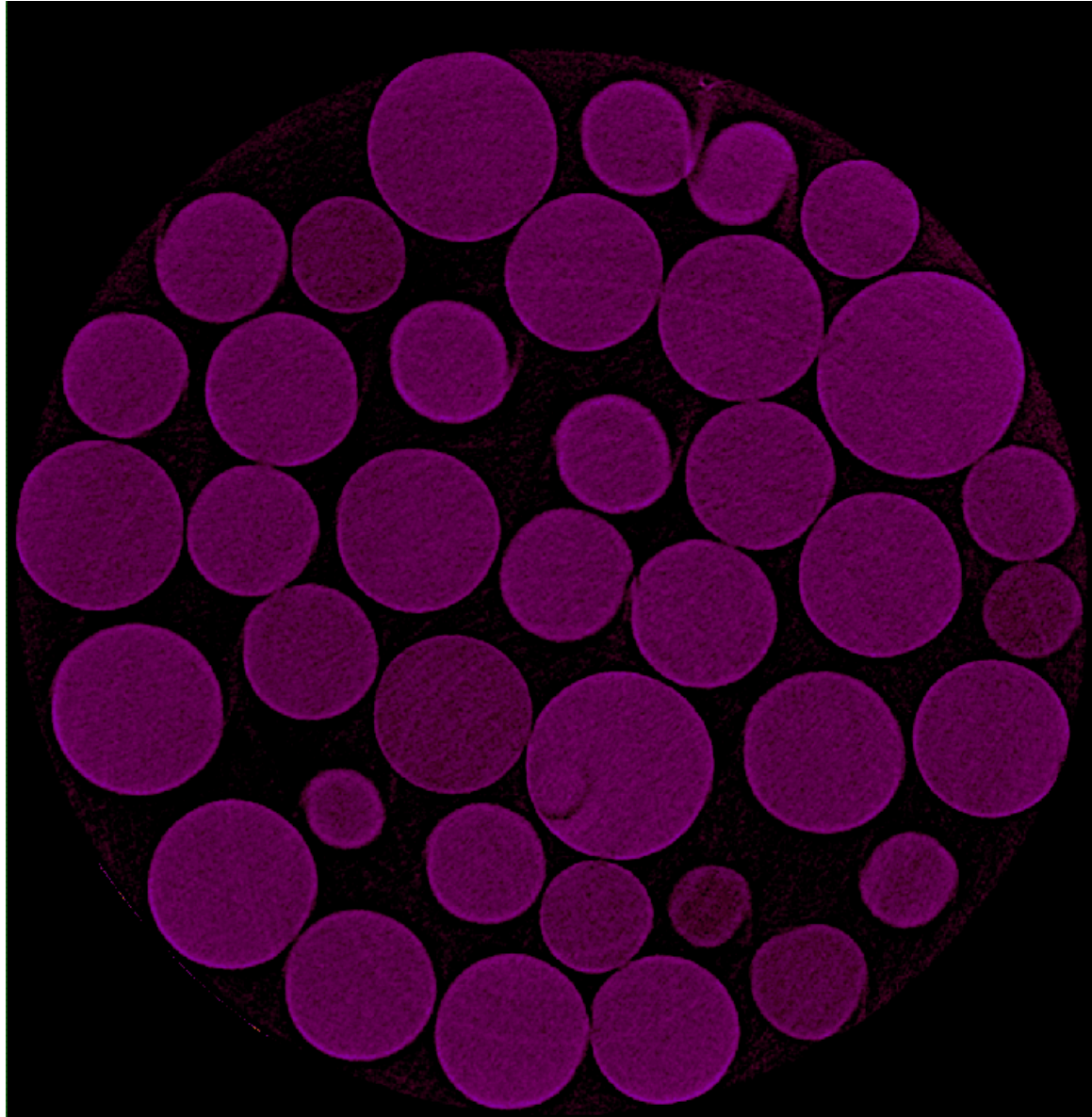* Slides 11: Trace Elemental analysis via Inductively Coupled Plasma – Atomic Emission Spectroscopy (IAP-AES)
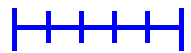
3M

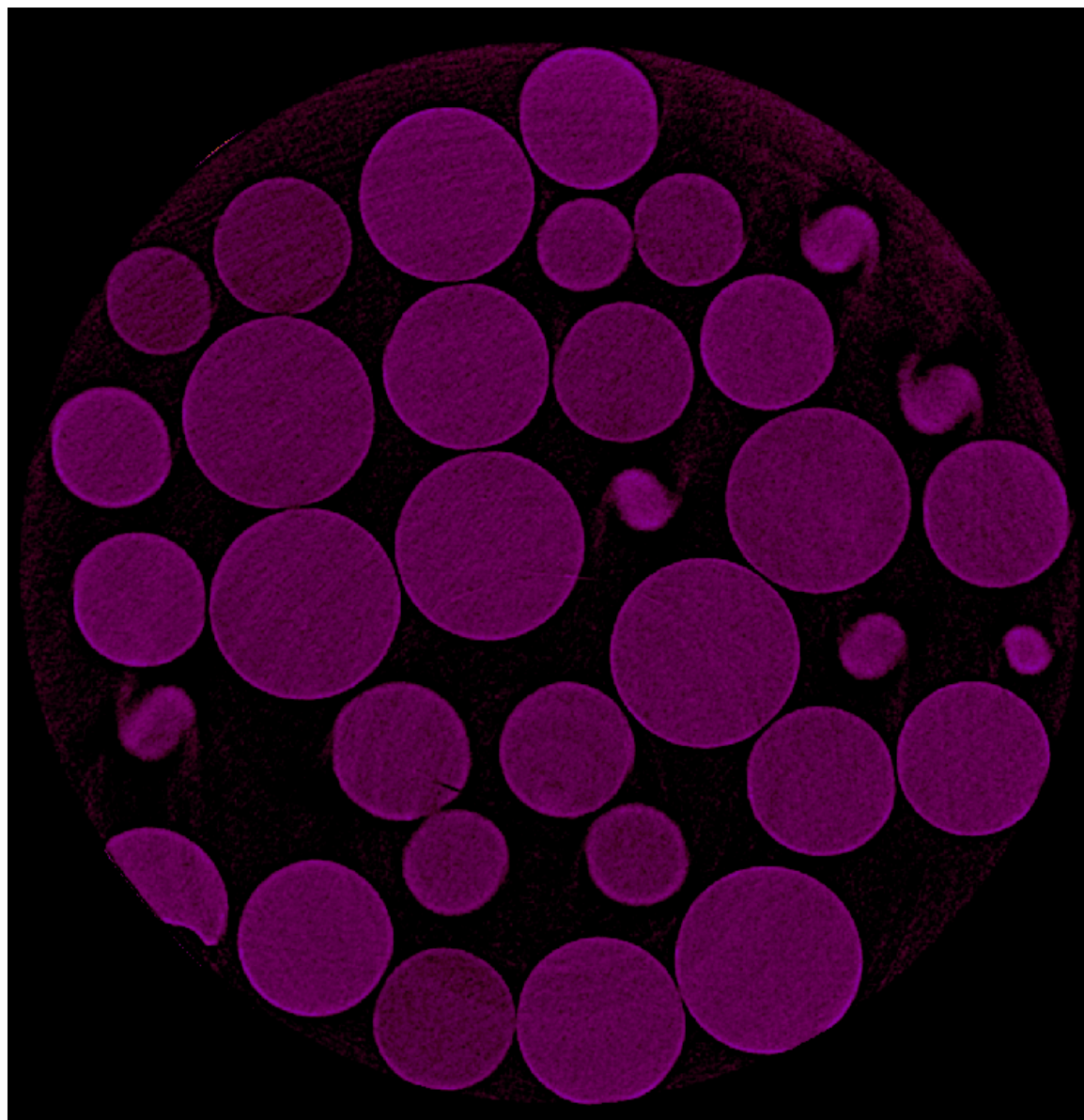# X-ray Diffraction and Tomography Studies (Slides 2-7)

(A) BAM-P108

(B) BAM-P109

reflection geometry WAXS data

3.8 Å

2.06 Å

1.2 Å

Intensity(Counts)

Two-Theta (deg)

3M CRAL

P109

500 μm

2D reconstructed slice

P109

500 µm

2D reconstructed slice

P109

500 µm

2D reconstructed slice

P109

500 μm

2D reconstructed slice

P109

Slice 1801

500 µm
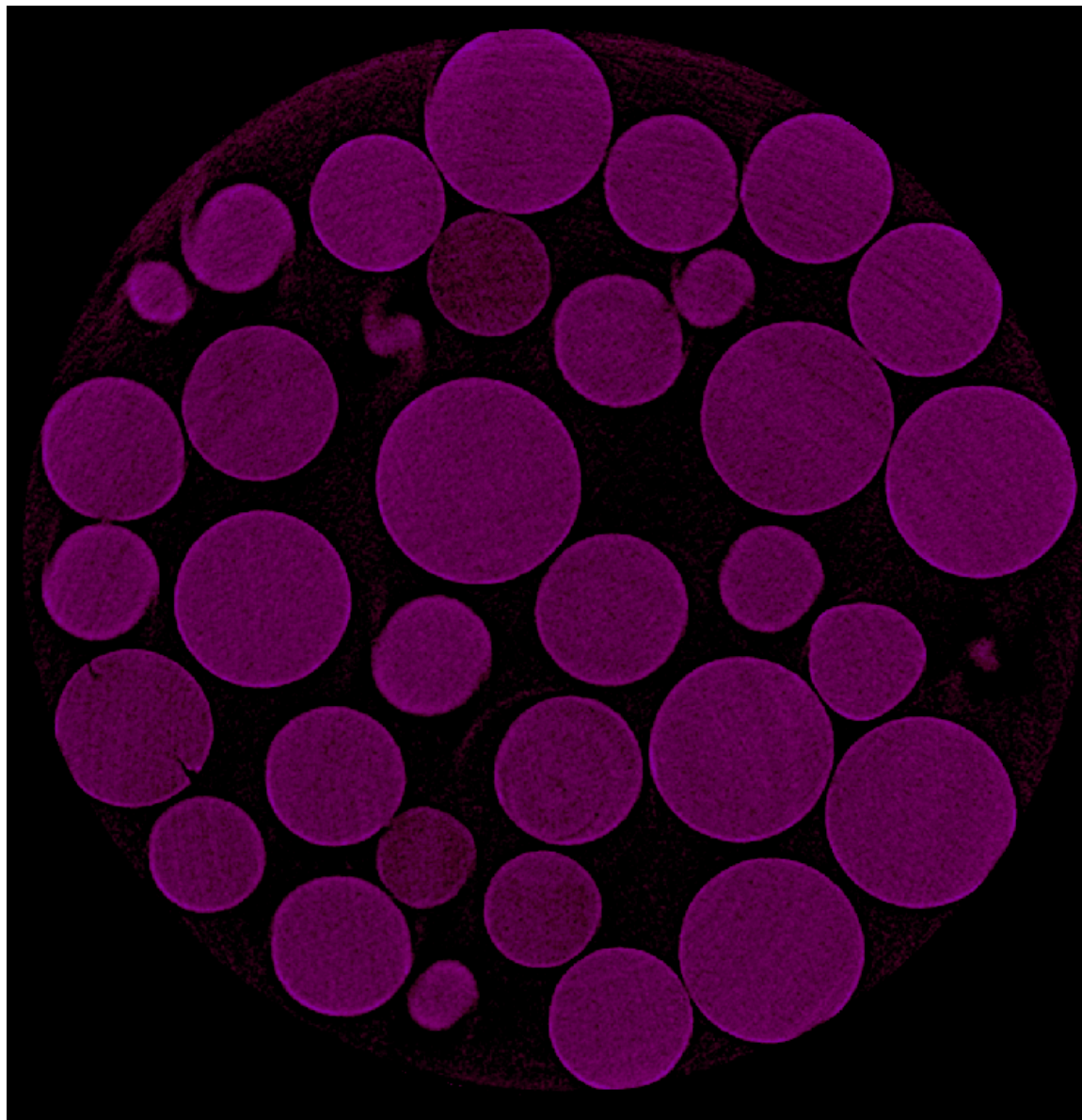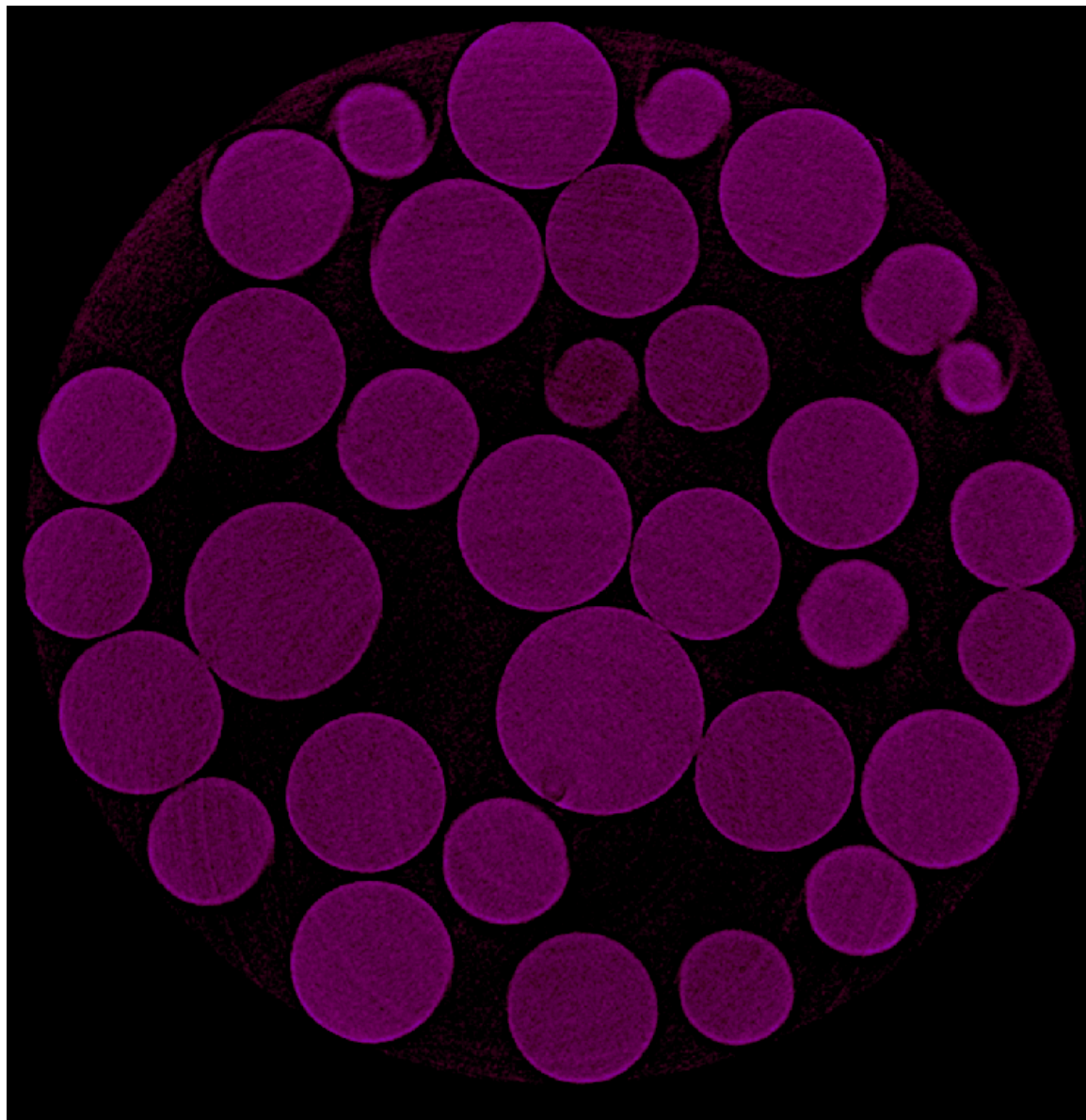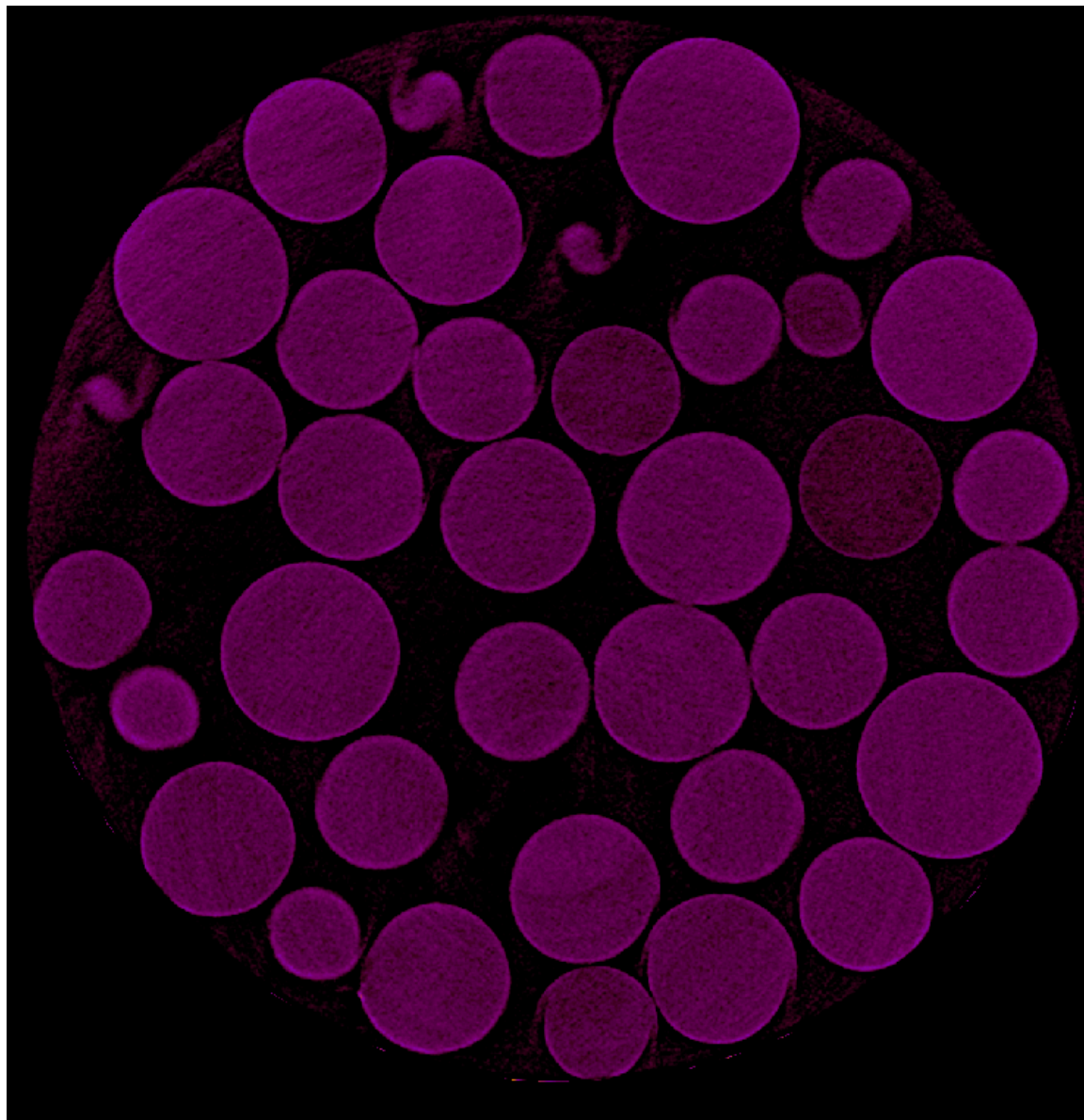
2D reconstructed slice

X-ray Photoelectron Spectroscopy – Slides 8-10

X-ray Photoelectron Spectroscopy – Slides 8-10

X-ray Photoelectron Spectroscopy – Slides 8-10

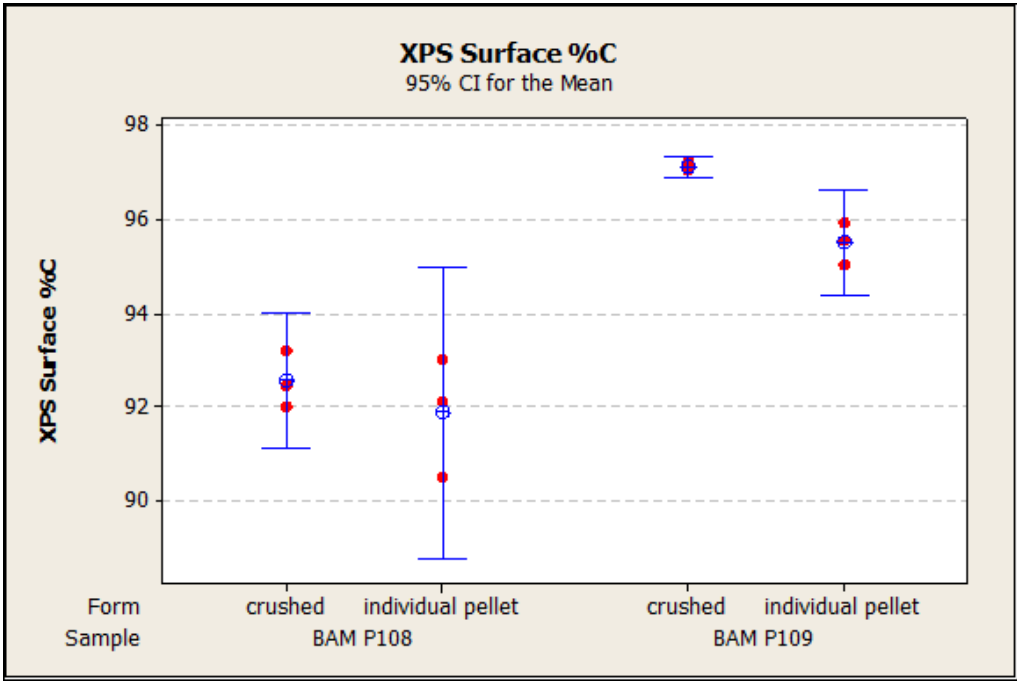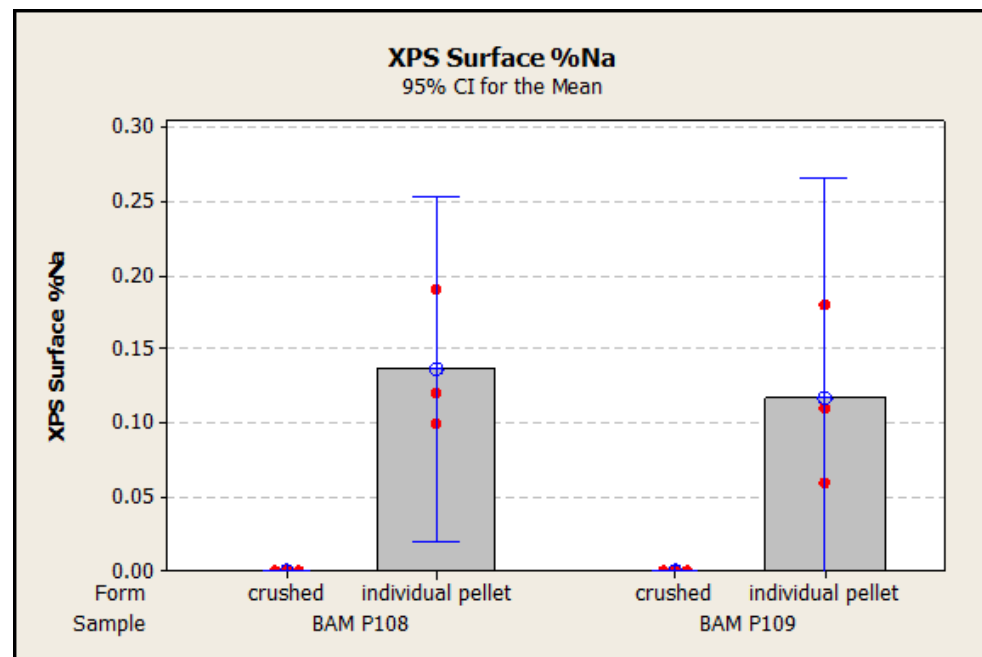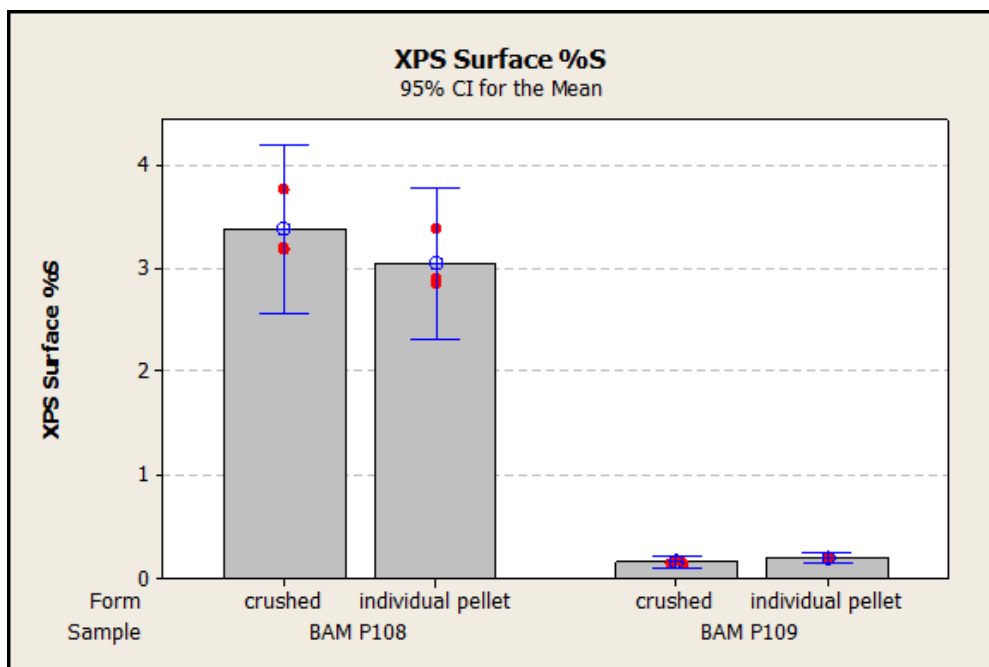| XPS Surface Concentrations (Atomic %)						
Sample	Form	Replicate	C	O	Na	S
BAM P108	crushed	A	92.0	4.2	0.0	3.8
BAM P108	crushed	B	92.5	4.3	0.0	3.2
BAM P108	crushed	C	93.2	3.6	0.0	3.2
BAM P108	individual pellet	A	93.0	4.0	0.1	2.9
BAM P108	individual pellet	B	90.5	6.4	0.2	2.9
BAM P108	individual pellet	C	92.1	4.4	0.1	3.4
BAM P109	crushed	A	97.2	2.6	0.0	0.19
BAM P109	crushed	B	97.1	2.8	0.0	0.15
BAM P109	crushed	C	97.0	2.8	0.0	0.15
BAM P109	individual pellet	A	95.6	4.1	0.1	0.22
BAM P109	individual pellet	B	96.0	3.8	0.1	0.18
BAM P109	individual pellet	C	95.0	4.6	0.2	0.21

3M

Trace Elemental analysis via Inductively Coupled Plasma – Atomic Emission Spectroscopy (IAP-AES)

Summary: A variety of trace elements were detected by ICP-AES. Of the 22 trace elements determined, the most abundant were sodium, calcium, and iron.

Element	Concentration (ppm) #1: BAM-P-108	Concentration (ppm) #2: BAM-P-109
Al	< 3	< 3
Ca	16 ± 1	24.7 ± 0.4
Cd	< 0.2	< 0.2
Co	< 0.1	< 0.1
Cr	0.4 ± 0.1	0.59 ± 0.05
Cu	0.19 ± 0.01	2.1 ± 0.1
Fe	14.9 ± 0.2	20.9 ± 0.5
K	< 4	< 4
Li	< 0.3	< 0.3
Mg	2.4 ± 0.2	3.6 ± 0.3
Mn	0.36 ± 0.02	1.35 ± 0.01
Mo	< 0.9	< 0.9

Explanation of Results:
The results reflect the average analyte concentrations (ppm, or μg/g). The concentrations have been corrected for impurities in the acid blanks. An entry marked with a "<" symbol indicates that the concentration is less than the specified detection limit. The reported uncertainties are one standard deviation of the duplicate measurements.

3M