

**Summary Statistics for TA_LP03_130703:
Micro-CT Data Acquired at LLNL, Specimen 3 of 4**

Isaac M. Seetho, Kenn E. Morales,
W. Travis White, III, Harry E. Martz, Jr.
Lawrence Livermore National Laboratory
Livermore, CA 94551

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Executive Summary

TA_LP03_130703				
Measured Density: 0.77 g/cm ³		X-ray tube voltages (source filter materials)		
Parameter		μ_L 100 kV(Al), Al-BHC	μ_L 100 kV(Al), H ₂ O-BHC	μ_H 160 kV (AlCu)
LAC	Mean Measured LAC (LMHU) ¹	1100	1110	752
	Standard Deviation/Mean	41%	37%	34%
	Entropy	7.52	7.44	6.96
$^L Z_{eff}$	From the mean measured LACs	7.79		
$^{LW} Z_{eff}$	From the mean measured LACs	7.28		
μ_L/μ_H	Using Al-BHC	1.46		
μ_L/μ_H	Using H ₂ O-BHC	1.48		
QA	From Cu strip and References	Pass		

Table 1. First-order statistics of the x-ray linear attenuation coefficient (LAC) in TA_LP03_130703, the estimated value of the effective atomic number, Z_{eff} [1] and μ_L/μ_H . Z_{eff} is calculated from the ratio of μ_L/μ_H . Beam hardening compensation has been applied to μ_L using both aluminum ($^L Z_{eff}$) and water ($^{LW} Z_{eff}$) beam hardening parameters.

Using x-ray micro computed tomography (MicroCT), we have characterized the linear attenuation coefficients (LAC), μ , of a sample of a dry powder material, tartaric acid (TA). specimen was prepared at Lawrence Livermore National Laboratory (LLNL), loaded into a 60mL low density polyethylene (LDPE) bottle. After completed packing, the specimen was scanned following the protocol for MicroCT measurements under Test Plan 79 [2].

This particular specimen, TA_LP03_130703, recorded the bulk packing density (mass of sample divided by volume of sample) shown above. Three other preparations were made and analyzed [3-5]. We used the computer program IMGREC to reconstruct the CT images. The values of the key parameters used in the x-ray data capture and image reconstruction are given in this report. Additional experimental details may be found in the SOP [6] and a separate document [7]. To characterize the statistical distribution of LAC values in each CT image, we first isolated an ~80% region or segment of volume elements (“voxels”) lying completely within the sample, away from the walls of the container. We then calculated the mean value, standard deviation and entropy for (a) the high and low energy image segments and for (b) their digital gradient images². The statistics of the initial image of LAC values are called “first order statistics;” those of the gradient image, “second order statistics.” See Seetho [8] for details of the analysis used to obtain the numbers reported in this document.

¹ LMHU: “LLNL modified Hounsfield units with respect to water.” To obtain the LAC in LMHU for some material at any energy, we multiply by 1000 and divide by the LAC of water at an x-ray energy of 160 kV with aluminum and copper filters.

² A digital gradient image of a given image was obtained by taking the absolute value of the difference between the initial image and that same image offset by one voxel horizontally, parallel to the rows of the x-ray detector array.

Summary of TA_LP03_130703 X-ray Statistics

Report Date: December 11, 2013

Report Prepared by: Isaac Seetho
Typed or Printed Name

LLNL
Organization

QA: Isaac Seetho
Typed or Printed Name

LLNL
Organization

Material ID(s): TA_LP03_130703

Source		Collimator	Beam Hardening	Sample Preparation	X-ray Measurement	Linear Attenuation Coefficient (LAC)				
Bias (kV)	Filters		Number of slits	Parameter Source	Date	Date	Statistic	1 st order	2 nd order	
	Material	Thickness								
100	Al	1.943 mm	2	H ₂ O	7/1/2013	7/3/2013	Mean	1110	752	
							Std. Dev.	412	256	
							Entropy	7.44	6.96	
100	Al	1.943 mm	2	Al	7/1/2013	7/3/2013	Mean	1100	307	
							Std. Dev.	451	231	
							Entropy	7.52	6.70	
160	Al Cu	1.943 mm 1.905 mm	2	None	7/1/2013	7/3/2013	Mean	282	175	
							Std. Dev.	211	132	
							Entropy	6.61	6.14	
^L Z _{eff}	Based on measured LAC (Al-BHC)								7.79	
^{LW} Z _{eff}	Based on measured LAC (H ₂ O-BHC)								7.28	
μ_L/μ_H	Based on measured LAC (Al-BHC)								1.46	
μ_L/μ_H	Based on measured LAC (H ₂ O-BHC)								1.48	

Table 2. Key statistics [9] for x-ray measurements of Linear Attenuation Coefficient (LAC). ^LZ_{eff} is determined from 100 kV (Al) to 160 kV (AlCu) LAC (μ_L/μ_H) as given in reference [1]. The statistics here are from the 2-slit image data (not the 1-slit open image data).

Comments: _____

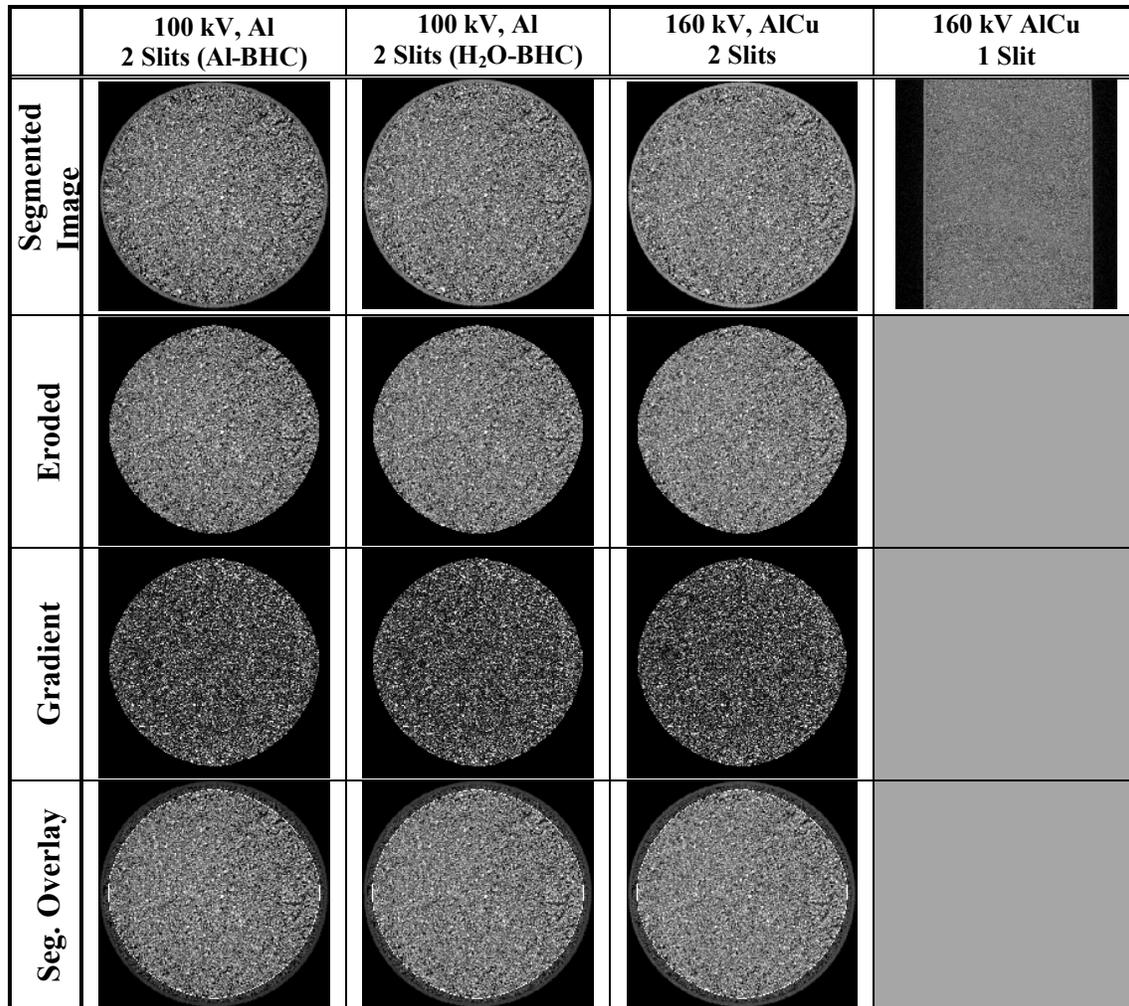


Figure 1. X-ray slice images with $150\mu\text{m} \times 150\mu\text{m} \times 150\mu\text{m}$ voxels. Raw data (top row), segmented images (second row), eroded images (third row) used to calculate first order statistics. Fourth row, difference or gradient image used for second-order statistics. Images not to scale and use different gray scales to obtain maximum contrast. Single slit images (top right) are used for a qualitative visual assessment of homogeneity.

Comments/Observations on Appearance of Sample (texture, color, other):

The specimen displays a generally uniform granulated texture.

SUPPLEMENTAL ANALYSIS

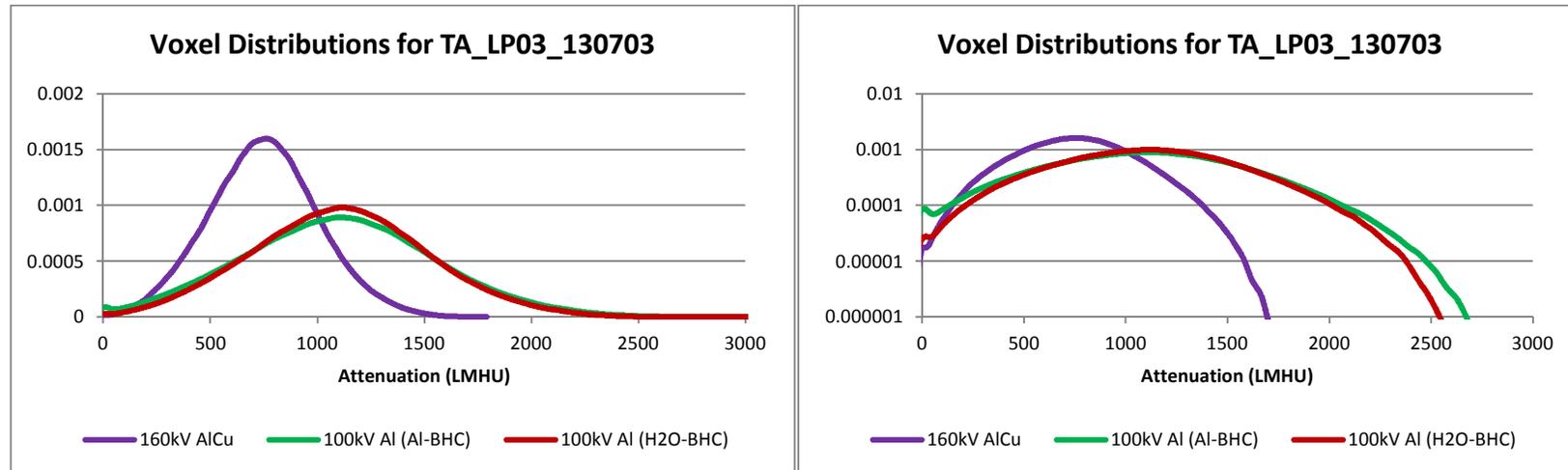


Figure 2. KDE histograms of values of the linear attenuation coefficient (LAC) for TA_LP03_130703 for two x-ray source settings (linear plots – left; semi-log plots – right).
Comments/Observations on Histograms: These histograms are made with a Gaussian Kernel Density Estimator (KDE) [9, 10] using 150- μ m voxel upper-slit CT images.

Reference Specimens

	Parameter	<i>graphite</i>	<i>ethanol</i>	<i>Delrin</i> *	<i>water</i>	<i>Teflon</i> **	<i>aluminum</i> ***
100kV, Al (Al-BHC)	Mean (LMHU)	1738	1037	1810	1411	3049	7020
	Std Dev LMHU)	82	59	82	54	89	135
100kV, Al (H2O-BHC)	Mean (LMHU)	1852	1123	1941	1507	3177	6738
	Std Dev LMHU)	78	59	75	54	65	228
160kV, AlCu	Mean (LMHU)	1394	805	1339	1000	1923	2956
	Std Dev LMHU)	63	47	57	48	61	73

Table 3. Linear attenuation coefficients of six reference materials as measured simultaneously with TA_LP03_130703.

* Acetron® GP copolymer. **Enflo Corp. PTFE. ***T6061 alloy.

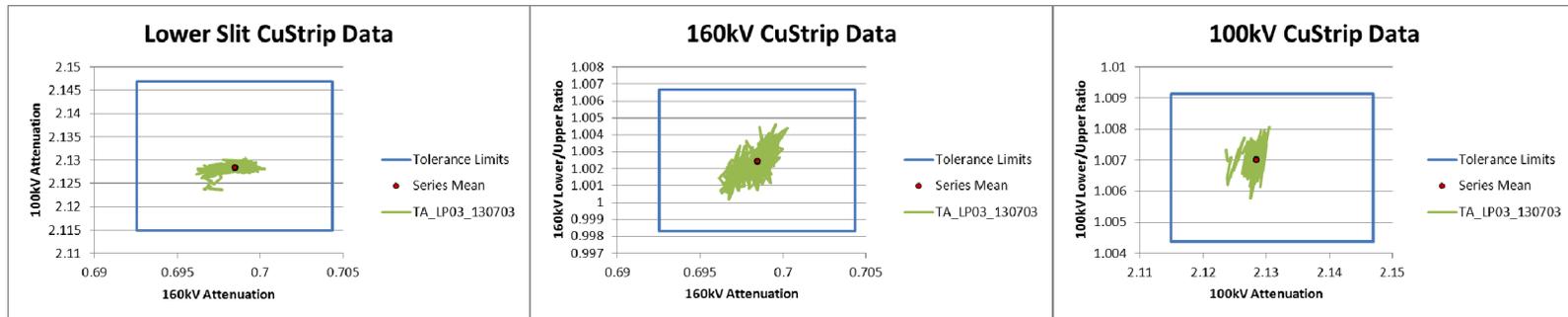


Figure 3. Copper strip data are within the defined tolerance limits. These tolerance limits were defined using a set of scans spanning from April through May 2013.

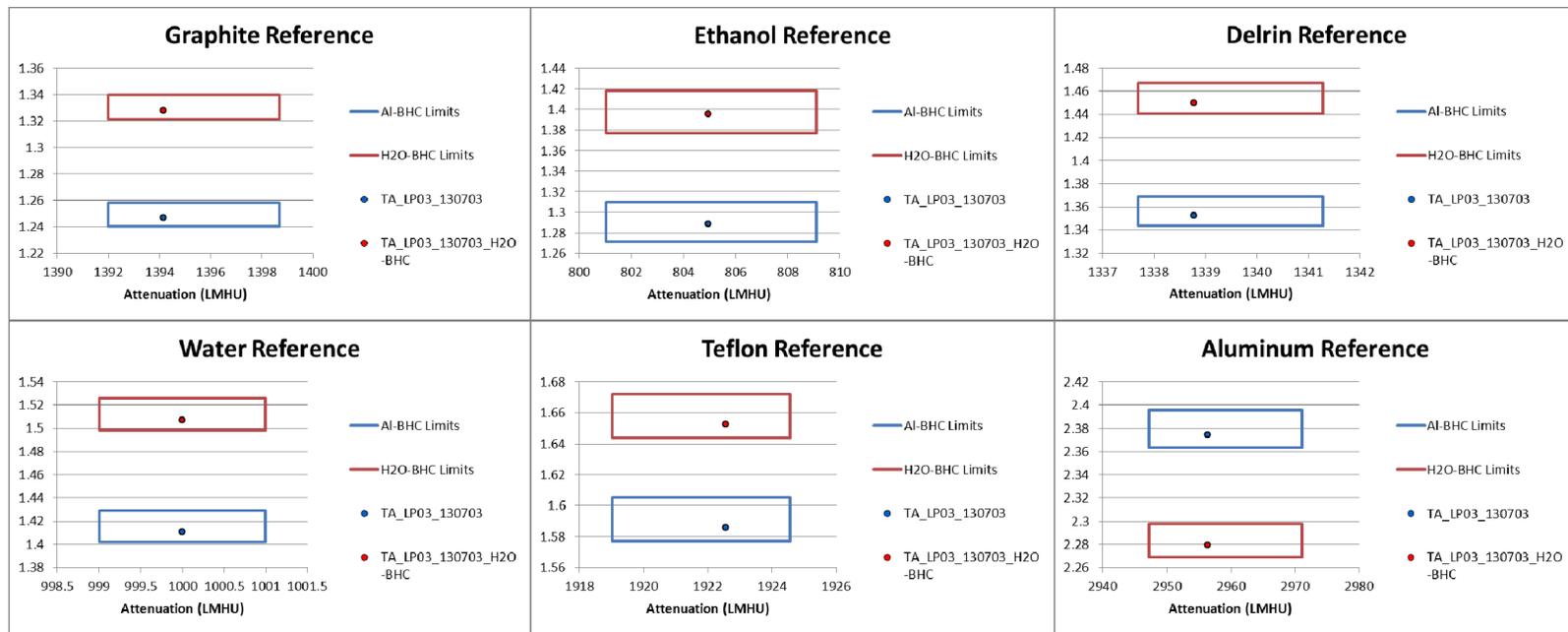


Figure 4. Reference materials are within the defined tolerance limits. These tolerance limits were defined using a set of scans spanning from April through May 2013.

Micro-CT System Configuration

1. Scan Location Site: LLNL HEAF
2. Source: Yxlon D09 450 kV Tube; Mfr. Catalog Number: 9421-172-33503; S/N 21-5204
3. Detector: Thales Flashscan 33 with Lanex Fine Gadolinium Oxysulfate Scintillator Screen; s/n 91106194
4. Rotation control system. Controller: Newport Model ESP7000 SN: 1250
5. Carousel: LLNL 2-tray, 6" Dia.
6. Data capture computer: Dell DHM/J4271

Micro-CT Scan Parameters

1. Scan Geometry:¹ SOD (mm): 1131.0 ODD (mm): 298.7
Number of positions: 400 Angular Range: 200° Angular Increment: 0.5°
2. Number of Frames averaged per Image: 4
3. Integration time per frame: See p 7.

¹ Distances are those recorded in the .sct file for this experiment and are the values used in image reconstruction.

File Storage Locations for X-ray Data

Specimen

Root Data Path:

\\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Test_Data\{sub directory}\

Specimen ID	Date	Radiographer	Slits	kV	mA	Al Filter (mm)	Cu Filter (mm)	Integration <i>dpix</i> Setting [time/frame (s)]	{sub directory}	File Name
TA_LP03_130703	130703	Morales	2	100	1.1	1.943	0	8 [2.8s]	TA_LP03_130703_100Al	TA_LP03_100Al_ <i>nn</i> .sdt ¹
	130703	Morales	2	160	4.35	1.943	1.905	8 [2.8s]	TA_LP03_130703_160AlCu	TA_LP03_160AlCu_ <i>nn</i> .sdt
	130703	Morales	1	160	4.35	1.943	1.905	8 [2.8s]	TA_LP03_130703_160AlCu1slit	TA_LP03_160AlCu1slit_ <i>nn</i> .sdt

Dark current, mid-range, bright field and I_o

Root Data Path:

\\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Test_Data\{sub directory}\

Slits	kV	Filter	{sub directory}	Dark Image File Name	Mid-Brightness Image File Name	Max Brightness Image File Name	I_o Image File Name
2	100	Al	TA_LP03_130703_100Al	TA_LP03_100AldrkR.sdt	TA_LP03_100AlmidR.sdt	TA_LP03_100AlIitR.sdt	TA_LP03_100Albak.sdt
2	160	AlCu	TA_LP03_130703_160AlCu	TA_LP03_160AlCudrkR.sdt	TA_LP03_160AlCumidR.sdt	TA_LP03_160AlCulitR.sdt	TA_LP03_160AlCubak.sdt
1	160	AlCu	TA_LP03_130703_160AlCu1slit	TA_LP03_160AlCu1slitdrkR.sdt	TA_LP03_160AlCu1slitmidR.sdt	TA_LP03_160AlCu1slitlitR.sdt	TA_LP03_160AlCu1slitbak.sdt

¹ *nn* - is the CT angular index number (0 through 399) for each individual data file

Reconstruction

Reconstructed by: Kenneth E. Morales

Date: 7/3/2013

Location: LLNL

Computer: Dell Precision 690

Reconstruction Software

Software: IMGREC

Version: 2.8.1.1c11

Beam hardening compensation: Only for 100 kV Al filtered data using Al and H₂O reference materials for compensation.

Script Files

LLNL_script_TA_LP03_100Al.txt

LLNL_script_TA_LP03_160AlCu.txt

LLNL_script_TA_LP03_160AlCu1slit_tw_WDB.txt

LLNL_script_H2OBHC_TA_LP03_100Al.txt

Reconstructed Specimen Files

Root Data Path:

\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Reconstruction\
Recon_130703\{sub directory}\

Slits	kV	Filter	{sub directory}	Reconstruction file name
2	100	Al	TA_LP03_130703_100Al	recobj_nn ¹ .sdt
2	100	Al	H2O_Recon\TA_LP03_130703_100Al	recobj_nn.sdt
2	160	AlCu	TA_LP03_130703_160AlCu	recobj_nn.sdt
1	160	AlCu	TA_LP03_130703_160AlCu1slit	recry_nn.sdt , ry_nn.sdt

Observations: _____

¹ nn - is the index number for each reconstruction file, modified by an offset corresponding to the frame subsection extracted and analyzed.

Analysis

Analysis by: Isaac Seetho

Date: 7/3/2013

Location: LLNL

Computer: Dell Precision T7500

Analysis Software

Software: MATLAB

Version: R2010b

GUI Function/Script Files

micro_ct_gui_1_3.m¹

custrip_gui_split.m

Reference & Specimen Analysis Files

\\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Analyses\
TA_LP03_130703_analysis_IMS_130703\

Analysis File	TA_LP03_130703_characterization.xlsx
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\\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Analyses\TA_LP03_130703_H2O-
BHC_analysis_IMS_130703\

Analysis File	TA_LP03_130703_H2O-BHC_characterization_Corrected.xlsx
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Copper Strip Analysis Files

Root Data Path:

\\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LP03_130703\Analyses\
TA_LP03_130703_custrip_IMS_130703\

Aggregate Statistics	Stats_TA_LP03_130703_W80xH7.xls
Mean Value Time Series	Custrip_TA_LP03_130703_W80xH7.xls

¹ Analysis using the MicroCT GUI is done according to the steps outlined in reference [8].

REFERENCES

1. Jeffrey S. Kallman, Daniel J. Schneberk, Harry E. Martz, Jr., *Two-energy Ratio Method to Determine Zeff from Reference Materials: A Comparison of an Explosive and a Simulant*, Version 3, Lawrence Livermore National Laboratory, LLNL-TR-491153, June 24, 2011.
2. Stephen Azevedo, Jeffrey S. Kallman, Harry E. Martz, Jr., *TP79 – Microstructure Studies Using MicroCT and EDS for DHS R&D*, Lawrence Livermore National Laboratory.
3. Isaac M. Seetho, Kenn E. Morales, W. Travis White III, Harry E. Martz, Jr., *Summary Statistics for TA_LP01_130624: Micro-CT Data Acquired at LLNL, Specimen 1 of 4*, Lawrence Livermore National Laboratory, LLNL-TR-653591, December 11, 2013.
4. Isaac M. Seetho, Kenn E. Morales, W. Travis White III, Harry E. Martz, Jr., *Summary Statistics for TA_LP02_130702: Micro-CT Data Acquired at LLNL, Specimen 2 of 4*, Lawrence Livermore National Laboratory, LLNL-TR-653600, December 11, 2013.
5. Isaac M. Seetho, Kenn E. Morales, W. Travis White III, Harry E. Martz, Jr., *Summary Statistics for TA_LP04_130708: Micro-CT Data Acquired at LLNL, Specimen 4 of 4*, Lawrence Livermore National Laboratory, LLNL-TR-654452, December 11, 2013.
6. “Standard Operating Procedure — Industrial Computed Tomography System Data Collection of Home-Made Explosives,” U.S. Department of Homeland Security Science and Technology Directorate, DHS/STD/TSL-xx-xx, July 9, 2009.
7. Jerel A. Smith, Daniel J. Schneberk, Jeffrey S. Kallman, Harry E. Martz, Jr., David Hoey, *Documentation of the LLNL and Tyndall Micro-Computed-Tomography Systems*, Version 091216, Lawrence Livermore National Laboratory, LLNL-TR-421377, December 17, 2009.
8. Isaac Seetho, *MicroCT: Analysis of CT Reconstructed Data of Home Made Explosive Materials Using the Matlab MicroCT Analysis GUI*, Lawrence Livermore National Laboratory, IDD-MCT-SOP-007, January 13, 2011.
9. Harry E. Martz, Jr., and Carl Crawford, *Validation of Explosive Simulants Requirement Specification*, Version 12, Lawrence Livermore National Laboratory, LLNL-TR-416983-REV 1, October 26, 2009.
10. B. W. Silverman, *Density Estimation*, Chapman and Hall, 1986.