Summary Statistics for TA_LT04_130724: Micro-CT Data Acquired at LLNL, Specimen 3 of 3

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Executive Summary

TA_LT04_130724				
Measured Density: 0.9 **g/cm^3**		**X-ray tube voltages (source filter materials)**		
Parameter		μ_L 100 kV(Al), Al-BHC	μ_L 100 kV(Al), H_2O-BHC	μ_H 160 kV (AlCu)
LAC	*Mean Measured LAC (LMHU)*[1]	1215	1214	825
	Standard Deviation/Mean	37%	33%	30%
	Entropy	7.51	7.41	6.93
${}^{L}Z_{eff}$	*From the mean measured LACs*	7.86		
${}^{LW}Z_{eff}$	*From the mean measured LACs*	7.26		
μ_L/μ_H	*Using Al-BHC*	1.47		
μ_L/μ_H	*Using H_2O-BHC*	1.47		
QA	*From Cu strip and References*	See p.5		

Table 1. *First-order statistics of the x-ray linear attenuation coefficient (LAC) in TA_LT04_130724, 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). The 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_LT04_130724, recorded the bulk packing density (mass of sample divided by volume of sample) shown above. Two additional preparations were made and analyzed [3-4]. 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 [5] and a separate document [6]. 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 images[2]. The statistics of the initial image of LAC values are called "first order statistics;" those of the gradient image, "second order statistics." See Seetho [7] 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_LT04_130724 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_LT04_130724

Source			Collimator	Beam Hardening	Sample Preparation	X-ray Measurement	Linear Attenuation Coefficient (LAC)		
Bias (kV)	**Filters**		**Number of slits**	**Parameter Source**	**Date**	**Date**	**Statistic**	**1st order**	**2nd order**
	Material	**Thickness**							
100	Al	1.943 mm	2	H_2O	7/18/2013	7/24/2013	**Mean**	1214	276
							Std. Dev.	399	206
							Entropy	7.41	6.59
100	Al	1.943 mm	2	Al	7/18/2013	7/24/2013	**Mean**	1215	306
							Std. Dev.	444	228
							Entropy	7.51	6.69
160	Al Cu	1.943 mm 1.905 mm	2	None	7/18/2013	7/24/2013	**Mean**	825	172
							Std. Dev.	248	129
							Entropy	6.93	6.12
${}^{L}Z_{eff}$	**Based on measured LAC (Al-BHC)**							7.86	
${}^{LW}Z_{eff}$	**Based on measured LAC (H_2O-BHC)**							7.26	
μ_L/μ_H	**Based on measured LAC (Al-BHC)**							1.47	
μ_L/μ_H	**Based on measured LAC (H_2O-BHC)**							1.47	

Table 2. *Key statistics [8] for x-ray measurements of Linear Attenuation Coefficient (LAC). ${}^{L}Z_{eff}$ 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:

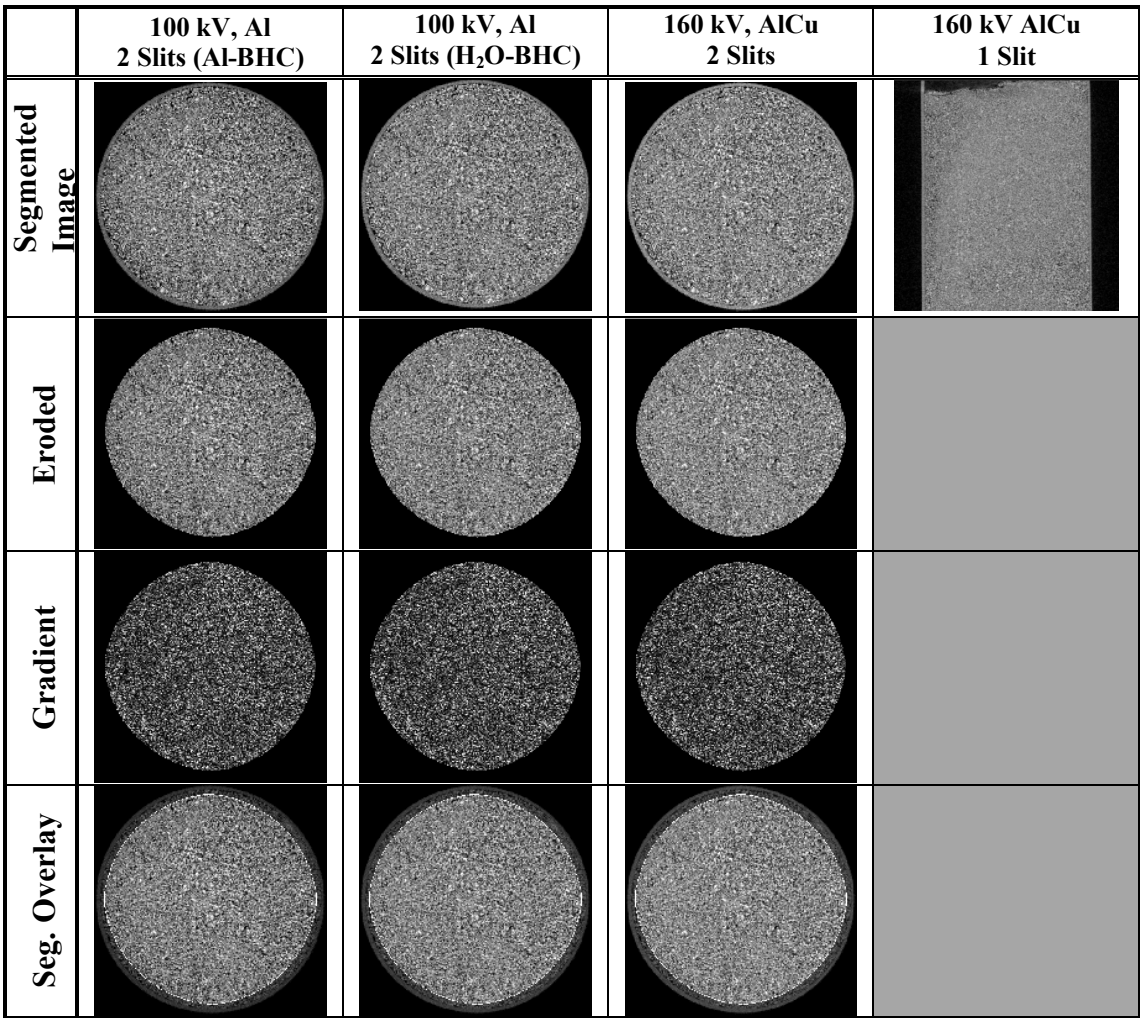

Figure 1. *X-ray slice images with 150µm × 150 µm × 150 µm voxels.* ***Raw data (top row), segmented images (second row), eroded images (third row) used to calculate first order statistics. Fourth row, difference or gradient image used for second-order statistics. Images not to scale and use different 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 appears to have a uniform granulated texture.

SUPPLEMENTAL ANALYSIS

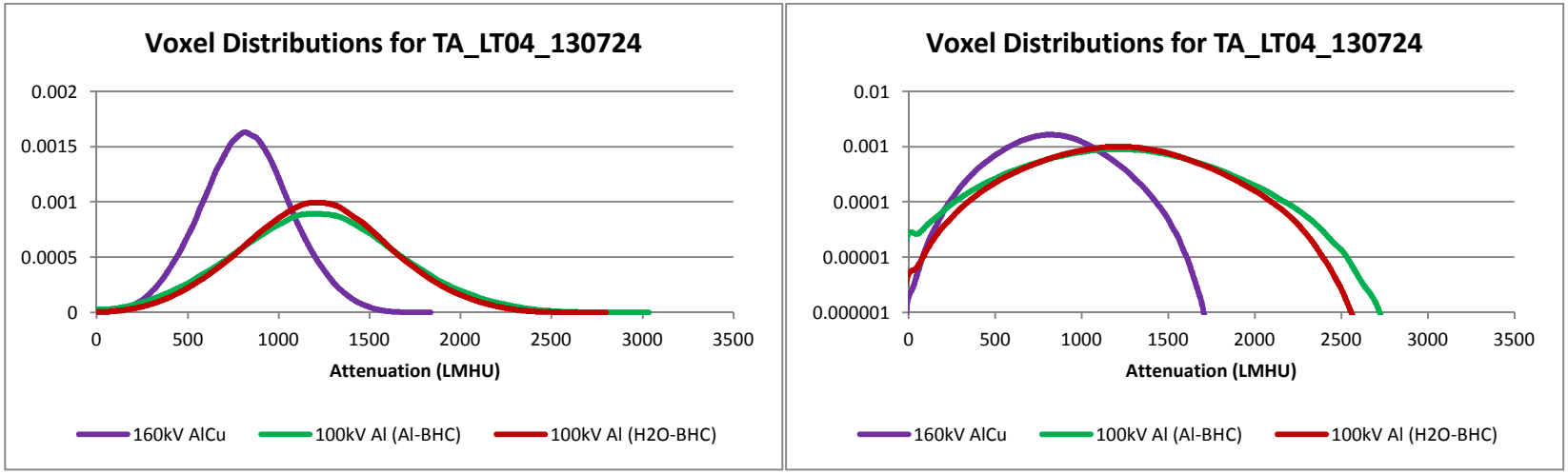

Figure 2. *KDE histograms of values of the linear attenuation coefficient (LAC) for TA_LT04_130724 for two x-ray source settings (linear plots – left; semi-log plots – right).*

Comments/Observations on Histograms: These histograms are made with a Gaussian Kernel Density Estimator (KDE) [8, 9] using 150-µm voxel upper-slit CT images.

Reference Specimens

	Parameter	*graphite*	*ethanol*	*Delrin**	*water*	*Teflon***	*aluminum****
100kV, Al (Al-BHC)	Mean (LMHU)	1736	1036	1807	1409	3039	6970
	Std Dev LMHU)	82	58	82	55	88	142
100kV, Al (H2O-BHC)	Mean (LMHU)	1851	1123	1939	1506	3170	6702
	Std Dev LMHU)	78	58	76	55	65	238
160kV, AlCu	Mean (LMHU)	1396	804	1339	1000	1922	2957
	Std Dev LMHU)	62	48	58	48	60	73

Table 3. *Linear attenuation coefficients of six reference materials as measured simultaneously with TA_LT04_130724.*

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

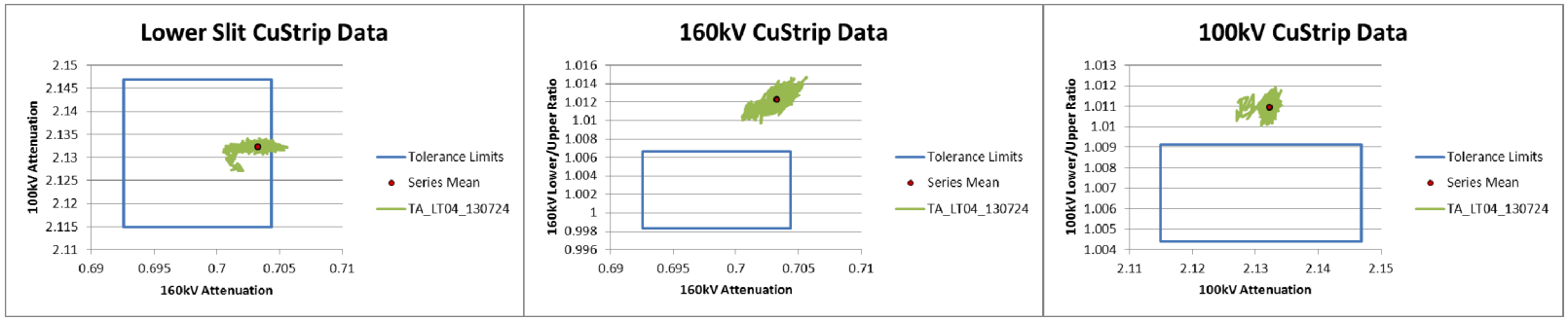

Figure 3. *Copper strip ratios for 160kV and 100kV are above limits. These tolerance limits were defined using a set of scans spanning from April through May 2013.*

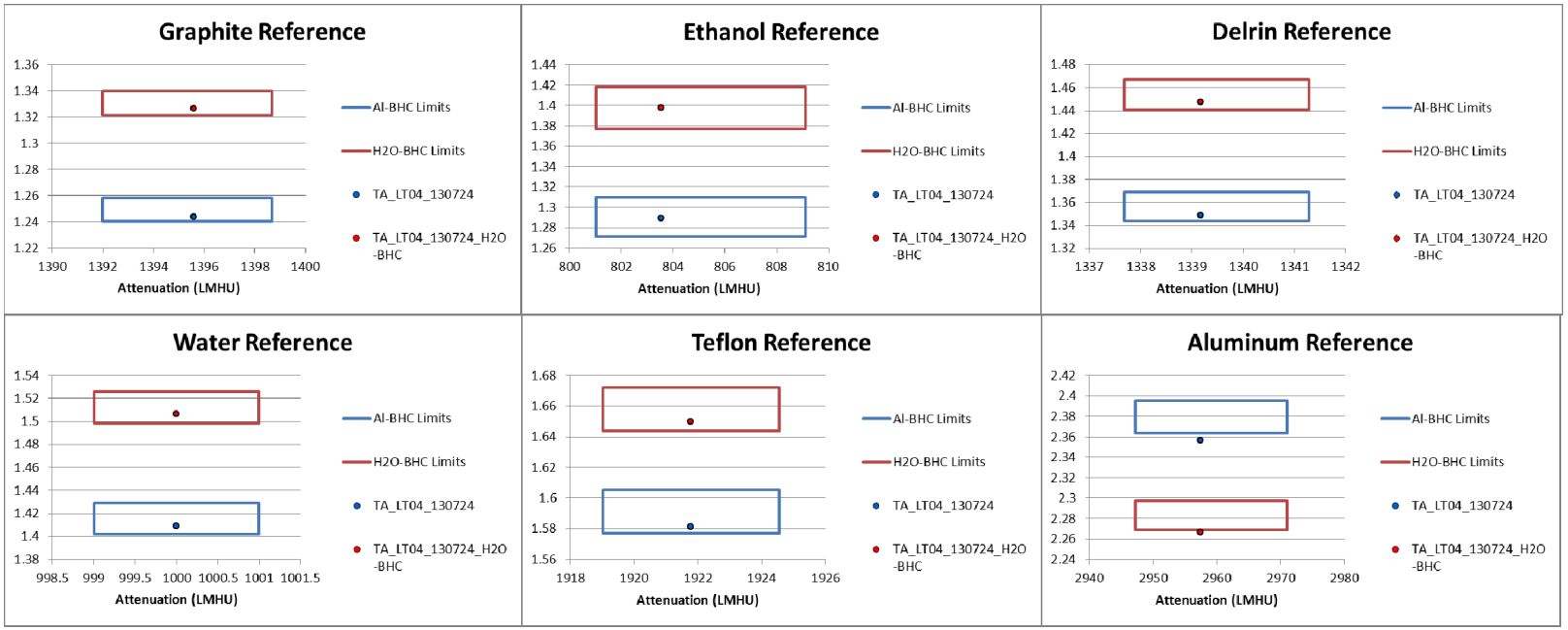

Figure 4. *Reference materials are within the defined tolerance limits, except for the aluminum ratio (which is just below bounds). These tolerance limits were defined using a set of scans spanning from April through May 2013.*

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_LT04_130724\Test_Data\{sub directory}\

Specimen ID	Date	Radiographer	Slits	kV	mA	Al Filter (mm)	Cu Filter (mm)	Integration *dpix* Setting [time/frame (s)]	{sub directory}	File Name
TA_LT04_ 130724	130724	Morales	2	100	1.1	1.943	0	8 [2.8s]	TA_LT04_130724_100Al	TA_LT04_100Al_*nn*.sdt[1]
	130724	Morales	2	160	4.35	1.943	1.905	8 [2.8s]	TA_LT04_130724_160AlCu	TA_LT04_160AlCu_*nn*.sdt
	130724	Morales	1	160	4.35	1.943	1.905	8 [2.8s]	TA_LT04_130724_ 160AlCu1slit	TA_LT04_160AlCu1slit_ *nn*.sdt

Dark current, mid-range, bright field and I_o

Root Data Path:

\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT04_130724\Test_Data\{sub directory}\

Slits	kV	Filter	{sub directory}	Dark Image File Name	Mid-Brightness Image File Name	Max Brightness Image File Name	*Io* Image File Name
2	100	Al	TA_LT04_130724_100Al	TA_LT04_100AldrkR.sdt	TA_LT04_100AlmidR.sdt	TA_LT04_100AllitR.sdt	TA_LT04_100Albak.sdt
2	160	AlCu	TA_LT04_130724_160AlCu	TA_LT04_160AlCudrkR.sdt	TA_LT04_160AlCumidR.sdt	TA_LT04_160AlCulitR.sdt	TA_LT04_160AlCubak.sdt
1	160	AlCu	TA_LT04_130724_ 160AlCu1slit	TA_LT04_ 160AlCu1slitdrkR.sdt	TA_LT04_ 160AlCu1slitmidR.sdt	TA_LT04_ 160AlCu1slitlitR.sdt	TA_LT04_ 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: 7/24/2013

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 H_2O reference materials for compensation.

Script Files

LLNL_script_TA_LT04_100Al.txt
LLNL_script_TA_LT04_160AlCu.txt
LLNL_script_TA_LT04_160AlCu1slit_tw_WDB.txt
LLNL_script_H2OBHC_TA_LT04_100Al.txt

Reconstructed Specimen Files

Root Data Path:
\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT04_130724\Reconstruction\Recon_130724\{sub directory}\

Slits	kV	Filter	{sub directory}	Reconstruction file name
2	100	Al	TA_LT04_130724_100Al	`recobj_`*nn*[1]`.sdt`
2	100	Al	H2O_Recon\TA_LT04_130724_100Al	`recobj_`*nn*`.sdt`
2	160	AlCu	TA_LT04_130724_160AlCu	`recobj_`*nn*`.sdt`
1	160	AlCu	TA_LT04_130724_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: 7/24/2013
Location: LLNL
Computer: Dell Precision T7500
Analysis Software
Software: MATLAB
Version: R2010b
GUI Function/Script Files
micro_ct_gui_1_3.m[1]
custrip_gui_split.m

Reference & Specimen Analysis Files

\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT04_130724\Analyses\TA_LT04_130724_analysis_IMS_130724\

Analysis File	TA_LT04_130724_characterization.xlsx

\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT04_130724\Analyses\TA_LT04_130724_H2O-BHC_analysis_IMS_130724\

Analysis File	TA_LT04_130724_H2O-BHC_characterization_Corrected.xlsx

Copper Strip Analysis Files

Root Data Path:
\Working\TP79_IMXXXXXX_Microstructure_Studies_V1\LLNL\None\HEAFCAT\None\TA_LT04_130724\Analyses\TA_LT04_130724_custrip_IMS_130724\

Aggregate Statistics	Stats_TA_LT04_130724_W80xH7.xls
Mean Value Time Series	Custrip_TA_LT04_130724_W80xH7.xls

[1] Analysis using the MicroCT GUI is done according to the steps outlined in reference [7].

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_LT02_130722: Micro-CT Data Acquired at LLNL, Specimen 1 of 3*, Lawrence Livermore National Laboratory, LLNL-TR-654472, December 11, 2013.
4. Isaac M. Seetho, Kenn E. Morales, W. Travis White III, Harry E. Martz, Jr., *Summary Statistics for TA_LT03_130723: Micro-CT Data Acquired at LLNL, Specimen 2 of 3*, Lawrence Livermore National Laboratory, LLNL-TR-654473, December 11, 2013.
5. "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.
6. 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.
7. 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.
8. 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.
9. B. W. Silverman, *Density Estimation*, Chapman and Hall, 1986.