Software Requirements Specification for ImgBeamer: SEM Image Formation

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Contents

Revision History

Date	Version	Notes
2023/02/03	1.0	First version
2023/02/11	1.1	Changes after review by domain expert
2023/02/1?	1.2	Changes after review by SRS secondary reviewer

1 Reference Material

This section records information for easy reference.

1.1 Table of Units

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

symbol	unit	SI
m	length	metre
s	time	second
Pa	pressure	pascal
J	energy	joule
K	temperature	kelvin
mol	substance	mole

Additional units used:

symbol	unit	name
px	pixel	picture element ?
nm	length	nanometre (10^{-9} m)
µm	length	micrometre (10^{-6} m)

1.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The choice of symbols was made to be consistent with the electron microscopy (EM) literature and with existing documentation for EM systems. The symbols are listed in alphabetical order.

symbol	unit	description
d_p	nm	probe diameter (size)
d_i	nm	probe step size in image space
d_o	nm	probe step size in object space
η	ratio	BSE yield
δ	ratio	SE yield

$I_{n \times m}$	8-bit gray level	Image intensity matrix that has n rows and m columns.
$M_{n \times m}$	boolean	Mask / stencil matrix that has n rows and m columns.
$R_{n \times m}$	8-bit gray level	Resulting image intensity matrix that has n rows and m columns.

1.3 Abbreviations and Acronyms

symbol	description
2D	two-dimensional
3D	three-dimensional
A	Assumption
BSE	Backscattered Electron
CCD	Charge Coupled Device
DD	Data Definition
EM	Electron Microscopy
FOV	Field of View
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
LM	Light Microscopy
PS	Physical System Description
R	Requirement
ROI	Region of Interest
SE	Secondary Electron
SEM	Scanning Electron Microscope
SRS	Software Requirements Specification
TM	Theoretical Model
ImgBeamer	SEM image formation demo tool

2   Introduction

Images formed by Scanning Electron Microscope (SEM) are created using a specific process where the image quality can be greatly influenced by the imaging parameters given by the user, aside from any inherent electron optics limitation of a given instrument. The motivation of this project is to be able to visualize qualitatively the influence of the spot profile (shape and size) and the raster parameters (such as pixel size). Since the quality of an image is very often evaluated subjectively by an experienced microscope user, the idea behind this software is providing a way to show that adjusting the imaging parameters could lead to a loss of information or misinterpretation. An underlying goal is also to prove or disprove if there is a "rule of thumb" for the optimal spot-to-pixel size ratio.

2.1   Purpose of Document

This document serves as the software specification. The details of the requirements, limitations, definitions, models to be used are laid explicitly within this document.

2.2   Scope of Requirements

The scope of the requirements of this software is restricted to only the image formation process used in SEMs, more specifically the image processing from signal to an image or visual representations. It does not cover election-sample interactions or CCD (charge coupled device) detector voltage to signal value conversion. See the assumptions section (Section 4.2.1) for further details.

2.3   Characteristics of Intended Reader

The intended reader of this document should have a basic understanding of electron-optics concepts used in an SEM. This can be equated to standard level two university physics (optics, electricity, magnetism, thermodynamics and modern physics) along with a standard undergraduate course related to materials characterization (concepts such as backscattered electrons, mean free path, and electron density). The reader should have a basic understanding of two-dimensional image processing techniques and level one university linear algebra (matrices).

2.4   Organization of Document

This document contains an introduction to the software and its goals. It is meant to be a reference document to the readers and is based on an SRS template from Smith and Lai (2005); Smith et al. (2007). The document includes a description of the scope, a detailed list of the terminology, definitions, and models used, as well as a more specific and detailed description of the problem and its solutions. This document also defines the requirements, as well as the likely changes and traceability details.

3 General System Description

This section provides general information about the system. It identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

3.1 System Context

The general input and output pattern of the ImgBeamer software is shown in the system context diagram (figure 1). This section also includes the responsibilities of the user and the software.
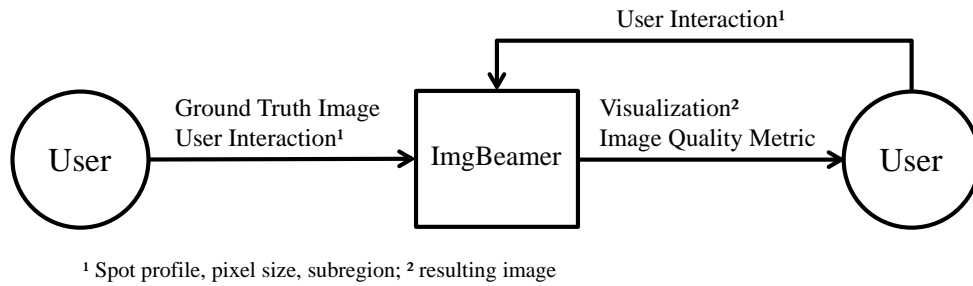

¹ Spot profile, pixel size, subregion; ² resulting image

Figure 1: System Context

- User Responsibilities:

  - Provide an image of sufficient size, such that the is enough visible detail.
  - Provided a ground truth image that should be free of distortions (e.g., from FOV edges, depth of field, "charging", insufficient focus, astigmatism, etc.).
  - Be able to interact with the software's graphical user interface using a computer mouse, keyboard and monitor.
  - Provide realistic spot profiles (size and shape).
  - Understand the basic concepts of the SEM image formation process.
  - Run the software on a platform or system with sufficient resources to process computer graphics.

- ImgBeamer Responsibilities:

  - Provide the ability load or change the input ground truth image.
  - Detect and warn about invalid or corrupt image files.
  - Set reasonable limits (minimum and maximum dimensions) on the spot profile.
  - Be responsive, taking user input at anytime and prevent locking or freezing of the graphical user interface as much as possible.

- Have reasonable starting default inputs and values.
- Display the image quality metric.
- Provide the ability to export the resulting images.

3.2 User Characteristics

The ImgBeamer software end user is anyone that has used an SEM or is learning about them. This ranges from a university undergraduate science student whose curriculum includes electron microscopy (EM), to experienced SEM operators or even to experts in the field of EM. The software end users also include those described in Section 2.3 (intended readers of this document). That said, image processing nor linear algebra knowledge is not required.

3.3 System Constraints

The real world design constraints are to be listed here, but currently this is none, or it is unknown if there are any.

4 Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models.

4.1 Problem Description

ImgBeamer is intended to help visualize and understand the influence of the spot profile and pixel size. It should be able to help determine the optimal spot-to-pixel-size ratio.

4.1.1 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

Terminology	Definition
Backscattered Electron	An electron that is elastically scattered backwards to the initial direction of travel as a result of electron-sample interactions between the beam and the sample.

Beam	The continuous focused stream of electrons accelerated at high speeds down the column of an electron microscope.
Bit Depth	It is the range of the value (intensity or color) of a pixel. Specifically, it is the maximum number of bits used to represent said value.
Brightness	The intensity value (or perceived luminance for colours) of a signal, point (or pixel), or area within an image.
Contrast	The difference or distinguishable quality of an intensity (or colour) or brightness value of a point (or pixel) from another point in an image.
Electron-Sample Interactions	The interactions as a result of electrons from the beam hitting the sample surface leading to an electron collision cascade. This in produces various emissions such as x-rays, BSEs, and SEs.
Electron Microscopy	The practice of microscopes that specifically use electrons as the source of illumination to produce an image or signal.
Exact-sampling	The sampling size or rate that matches the specificity of the targeted resolution. In the context of this document, this is when the size of the probe that matches the size of the pixel.
Field of View	The observable or visible extent given by the microscope and varies with magnification.
Ground Truth	The data or information that is considered as the source or reference standard of truth.
Image	A representation of visual information that can be represented by 2D matrix where each cell represents a pixel with a specific value (representative of intensity or colour). –
Image Quality	The perceived clarity, amount of information or detail representative of reality that is contained within an image.
Image Resolution	The size dimensions (width and height) of an image. Typically, it is defined in pixels.
Interaction Volume	The volume within the sample in which there are electron-sample interactions caused by the beam coming into contact with the surface of the sample.
Light Microscopy	The practice of microscopes that specifically use light as the source of illumination to produce an image or signal.
Mean Free Path	The average distance within a system that a particle can travel before it collides with other particles.
Nyquist Limit	More formally known as the "Nyquist-Shannon" sampling limit is the minimum sampling rate at which all the essential information is captured when discretizing a continuous signal, resulting in little to no distortions.

Over-sampling	This is a sampling rate or size that is too large where the specificity or origin of the information is lost. This generally results in increased confidence, but at a loss of precision.
Pixel Size	The size or dimensions of one cell within a raster grid.
Probe	Generally interchangeable with "beam". Contextually within this document, it is the final part of the beam that comes into contact with the surface of the sample (being analyzed within the microscope) forming a "spot" with a targeted size and shape.
Raster Grid	A scanning pattern with a defined and repeated cell size.
Region of Interest	A defined 2D area in both position, size, and shape on a sample.
Resolution	As defined by the Rayleigh criterion, it is the minimum distance by which two points or features can be distinguished.
Secondary Electron	An electron that emitted from the sample as a result of inelastic electron-sample interactions between the beam and the sample. These can be weakly bounded valence electrons or conduction band electrons.
Signal-to-Noise Ratio	The amount of information (signal) considered useful or representative of reality versus the amount of noise.
Spot Shape	The overall shape of the spot or probe, whether is it a perfect circle or elongated ellipse, or even a halo or ring.
Spot Size	The overall diameter or average feret/caliper diameter of the probe.
Step Size	The length or distance of a "pixel" by which the probe is moved or deflected when raster scanning the surface of a sample.
Subregion	A region or area contained within the current FOV.
Under-sampling	This is a sampling rate or size that is too small where the specificity or origin of the information is more restricted. This generally results in increased precision, but at a loss of confidence, or even accuracy.

4.1.2 Physical System Description

The basic principle of the SEM image formation process is to scan an electron beam over the surface of the sample (fig. 2) at discrete locations: cells of a raster or scan grid. A signal (e.g., BSEs, SEs) is produced as the beam dwells over each cell (representing a pixel in the resulting image). This signal is then collected by detectors to calculate a value (or intensity) to fill the corresponding pixel in the resulting image. The area sampled depends on the spot's (produced by the beam) size and shape (see fig 3).

The physical system of ImgBeamer, as shown in Figure 2 and 3, includes the following elements:

PS1: The sample that is being imaged or studied.

PS2: An SEM which includes a BSE and/or SE detector. The electron beam interacts with the sample surface in high-vacuum producing various signals.
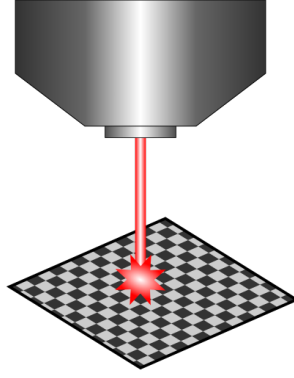
Figure 2: Schematic drawing of an electron beam hitting the sample surface within an SEM chamber. (Image from: https://github.com/joedf/ImgBeamer)
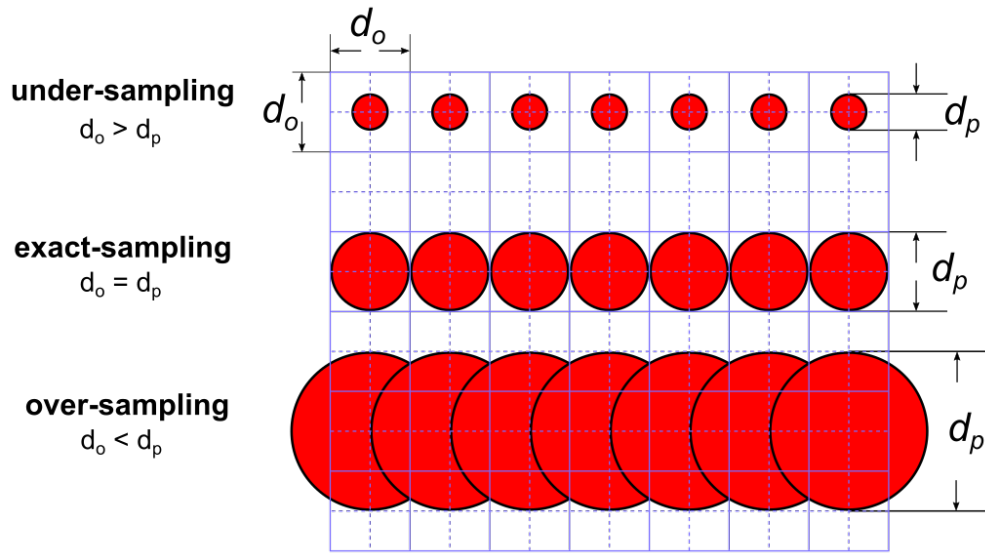

Figure 3: Schematic of the three sampling scenarios (under-sampling, exact-sampling, and over-sampling) and a visual representation of the pixel grid, d_p, and d_o. The dashed lines are to help visualize the center of each pixel cell. Adapted from Lifshin et al. (2014)

4.1.3 Goal Statements

Given an image (ground truth) and imaging parameters (e.g., spot size, spot shape, pixel size), the goal statements are:

GS1: Reprocess the image following the SEM image formation process.

GS2: Provide a quantitative metric of relative image quality of the resulting image.

GS3: Visualize the effects of changing the imaging parameters.

GS4: Export the reprocessed images.

4.2 Solution Characteristics Specification

This section provides the assumptions, instance models, theoretical models, general definitions, and data constraints. The information specified in this section is intended to reduce ambiguities and reduce the problem into clear logical or mathematical terms.

The instance models that govern ImgBeamer are presented in Subsection 4.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

4.2.1 Assumptions

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square brackets refer to the theoretical model [TM], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: The sample surface is solid.

A2: The sample surface is flat (meaning no topography).

A3: The sample surface is conductive (meaning no charge build up from electrons).

A4: The sample material is made of atoms with atomic numbers greater than 3 (lithium and lighter elements are not detectable in SEM).

A5: The electron beam is ideal (meaning stable and collimated meaning all the electrons are traveling parallel to each other down towards the sample surface within high vacuum for optimal mean free path).

A6: The beam intensity or current is considered uniform throughout the beam.

A7: The beam is orthogonal to the sample surface.

A8: The input image of the sample is considered to have infinite resolution representative of reality: ground truth.

A9: The signal yields (such as BSEs and SEs, see DD1) are high enough to produce an image meaning optimal SNR (enough signal and noise is low).

A10: The SEM is within a controlled environment: climate controlled (temperature and humidity) and low vibration room.

A11: The image produced by the SEM (see DD2) as the electron raster scan the sample surface is an approximate representation of reality.

4.2.2 Theoretical Models

This section focuses on the general equations and laws that ImgBeamer is based on.

Number	TM1
Label	**Mean Free Path**
Equation	$\lambda = \frac{RT}{\sqrt{2}\pi d^2 N_A P}$
Description	λ is the mean free path (m)
	R is the universal gas constant $= 8.3145$ J/mol K
	T is the temperature (K)
	d is the molecular diameter (m)
	P is the pressure (Pa)
	N_A is Avogadro's number $= 6.0221 \times 10^{23}$ mol^{-1}
Notes	See A5.
Sources	http://hyperphysics.phy-astr.gsu.edu/hbase/Kinetic/menfre.html
Ref. By	–

Number	TM2
Label	**Contrast**
Equation	$C_{tr} = (S_{max} - S_{min})/S_{max}$
Description	S is the emitted signal strength or intensity (see DD1).
Notes	$S_{max} > S_{min}$
Sources	Goldstein et al. (2018b), Lifshin et al. (2014)
Ref. By	–

Number	TM3
Label	**Magnification**
Equation	$M = \frac{d_i}{d_o}$
Description	M is the magnification ratio (unitless)
	d_i is the probe step size in image space
	d_o is the probe step size in object space
Notes	The input (ground truth) should be large enough and sufficient detail, see A8.
Sources	Lifshin et al. (2014)
Ref. By	–

4.2.3 General Definitions

This section collects the laws and equations that will be used in building the instance models.

Number	GD1
Label	**Raster or Scan Grid**
Units	nm, µm, or px (pixels)
Equation	$G(x, y) : \{x \geq 0, y \geq 0\}$
Description	This is a grid pattern applied to the sample surface within the FOV and spanning within deflection space (GD2) of the SEM.
	Each cell is a discrete x-y location over which the beam scans over to produce a signal. These signals are then collected by detectors to generate an image.
	Each cell represents a picture element or "pixel" that is by convention square.
	Non-square pixels may lead to unfaithful or distorted representations, see A11.
Source	Goldstein et al. (2018a)
Ref. By	–

Number	GD2
Label	**Deflection Space (or area / field)**
Description	The deflection space is the area bounds in which the beam can be redirected or oriented using deflection coils. It can be expressed in real world units, but this can vary between SEMs.
	From an imaging perspective, it can be generalized as a normalized unit square coordinate system where the top left is (-0.5, -0.5), the center is (0.0, 0.0), and the bottom right is (0.5, 0.5).
Source	Goldstein et al. (2018a)
Ref. By	–

4.2.4 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.

Number	DD1
Label	**Signal yield / intensity**
Symbol	η (for BSE), δ (for SE), Y (for general)
Units	ratio - unitless
Equation	$Y_{signal} = N_{signal}/N_B$
Description	Y_{signal} is the intensity relative to the incident beam.
	N_{signal} is the number of scattered or emitted electrons.
	N_B is the number of (primary) incident electrons from the beam.
Notes	The *signal* can BSE or SE.
	There assumptions related to the beam, the signal produced, and sample nature, see A5, A9, A4.
Sources	Goldstein et al. (2018b)
Ref. By	DD2, T2, A9

Number	DD2
Label	**Signal Image**
Symbol	$I_{n \times m}$
Units	intensity / ratio - unitless
Description	Each cell represents a pixel with a signal intensity (see DD1) or brightness value where the range depends on the bit depth.
	A bit depth of 8 is 0 to 255 (0xFF), and 16 is 0 to 65535 (0xFFFF).
	We assume (see A9) there's enough signal that can be detected, as a 0 represents no or "undetected" signal.
Sources	Goldstein et al. (2018b)
Ref. By	IM1, A11

4.2.5 Instance Models

This section transforms the problem defined in Section 4.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 4.2.4 to replace the abstract symbols in the models identified in Sections 4.2.2 and 4.2.3.

The goal of reprocessing an image GS1 will be solved by IM1. The goal of providing an image quality metric will be solved by IM2.

Number	IM1
Label	**Bit BLT (as known as Bit Block Transfer)**
Input	an image $I_{n \times m}$ and a mask $M_{n \times m}$
Output	reprocessed image $R_{n \times m}$
Description	Given an image (see DD2) and mask (or stencil), a boolean operation is performed iteratively on each cell of the image matrix, based on the corresponding cell value found in the mask matrix at row i and column j.
	If the mask cell value (at i, j) is true (or any non-zero value), the corresponding image cell value is transferred/kept in the resulting/destination matrix.
	Otherwise, if the corresponding matrix cell (at i, j) is false (or zero), then no value is transferred, and zero will be inserted at i, j in the destination image matrix.
Sources	Pike et al. (1984), https://en.wikipedia.org/wiki/Bit_blit
Ref. By	R6

Number	IM2
Label	**Image quality metric / evaluation**
Input	an image $I_{n \times m}$ serving as ground truth and the image $R_{n \times m}$ to compare
Output	a positive ratio value ranging from 0 to 1.00.
Description	Given the original image (ground truth, see A8) and a reprocessed image, a metric must be calculated to express image similarity where 1.00 means a perfect match and 0.00 means absolutely no correlation or similarity found. If the images do no match in size, the smaller (or larger?) image shall be scaled to match. The values do not need to be absolutely quantitative. They only need to be relatively comparable when only changing d_p or the spot shape.
Sources	
Ref. By	R7, NFR2

4.2.6 Input Data Constraints

Table 2 shows the data constraints on the input output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The column for software constraints restricts the range of inputs to reasonable values. The software constraints will be helpful in the design stage for picking suitable algorithms. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise.

The specification parameters in Table 2 are listed in Table 3.

4.2.7 Properties of a Correct Solution

Not applicable, as this is visualization software where the correct or appropriate solution is determined by the user's satisfaction and desired results.

Table 2: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value	Uncertainty
d_p	$d_p > 0.4$ nm	$d_{min} \leq d_p \leq d_{max}$	10 nm	10%
d_i	$d_i > 0.4$ nm	$d_{min} \leq d_i \leq d_{max}$	150 nm	10%
$I_{n \times m}$	–	$n_{min} \leq n \leq n_{max}$	1024	10%
...	–	$m_{min} \leq n \leq m_{max}$	1024	10%
$I_{i,j}$	–	$0 \leq I_{i,j} \leq I_{max}$	128	10%

Table 3: Specification Parameter Values

Var	Value
d_{min}	0.4 nm
d_{max}	1000 nm
n_{min}	256 px
m_{min}	256 px
n_{max}	4096 px
m_{max}	4096 px
I_{max}	255 (8 bit depth)

5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

5.1 Functional Requirements

R1: Accept an input image in the following formats:

- PNG (Portable Net Graphics)
- JPG (Joint Photographic Experts Group)
- BMP (Bitmap)

– preloaded example images

R2: Accept user input of the spot profile (size and shape) and ensure that all its defining values are positive real numbers.

R3: Accept user input of pixel size and ensure it is a positive real number.

R4: Accept user input to specify a subregion (FOV) for processing.

R5: Display a representative spot layout used for processing the image.

R6: Reprocess (using IM1) and display the resulting image to the user.

R7: Calculate and display an image quality metric (according to IM2) to the user.

5.2 Nonfunctional Requirements

The key nonfunctional requirements of this software are accuracy, usability, maintainability, and portability. These are listed below in detail:

NFR1: **Accuracy** The images produced should be not manipulated to produce results that subjectively represent the opinions of the author(s) or developer(s). Thus, the software should transparently follow the specifications and be verifiable by an expert (see A11) in field. The trends in image quality metric (see IM2) are more important the metric values themselves.

NFR2: **Usability** The user should be able to intuitively use the software and quickly understand what is being displayed. There should be little to no setup required. The software should be user-friendly and straight forward to use. Although the intended use is more of a qualitative nature, the user should be able to grasp any trends in the change of the image quality metric (see IM2) when the input parameters are changed. The software should have a simple user interface and be responsive when given a relatively small input image (see input data constraints). A user survey may be conducted to ascertain the software's usability.

NFR3: **Maintainability** The code should follow a consistent style and be reasonably separated in multiple files were it makes sense. Function names should be no longer than 40 characters. Duplicate code should be avoided wherever possible. Comments should be plentiful, but short, and avoid any unnecessary use jargon or domain-specific terms.

NFR4: **Portability** The software should be cross-platform (Windows, Linux, MacOS) with little to no setup required. This can be in the form of a web-application in an HTML5 compliant web-browser.

6   Likely Changes

Here are changes listed that will likely be implemented as the software is improved.

LC1: Give a sense of scale in real world units such as nm. The user have to provide the physical dimension of the input image.

LC2: Simulate basic noise (such as Gaussian or Poisson) at an intensity defined by the user.

LC3: Provide the choice of different image quality metric algorithms.

7   Unlikely Changes

LC4: Processing multi-spectrum or multichannel images.

LC5: Simulate electron beam physics, collision cascades, sample nature, topography, or electron-sample interactions.

8   Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an "X" may have to be modified as well. Table 5 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 6 shows the dependencies of instance models, requirements, and data constraints on each other. Table 4 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11
T1					X						
T2											
T3								X			
GD1											X
GD2											
DD1				X	X				X		
DD2											X
IM1											
IM2								X			
LC1											
LC2											
LC3											
LC4								X			
LC5	X										

Table 4: Traceability Matrix Showing the Connections Between Assumptions and Other Items

	T1	T2	T3	GD1	GD2	DD1	DD2	IM1	IM2
T1									
T2									
T3									
GD1									
GD2				X					
DD1							X		
DD2								X	
IM1							X		
IM2									

Table 5: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM1	IM2	R1	R2	R3	R4	R5	R6	R7	NFR1	NFR2	NFR3	NFR4
IM1													
IM2									X	X	X		
R1													
R2													
R3													
R4													
R5													
R6	X												
R7	X												
NFR1													
NFR2													
NFR3													
NFR4													

Table 6: Traceability Matrix Showing the Connections Between Requirements and Instance Models

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