A Guide to the “X-ray Map Simulator” Tool in Lispix
The Lispix “X-ray Map Simulator” is a visibility predictor

- With quantitative elemental x-ray mapping becoming an increasingly attractive tool, we need to understand the limitations for a particular measurement situation, e.g.,
  1. How many counts per pixel are needed to recognize a compositional feature?
  2. How does feature size relative to image frame matter?
  3. For the particular element and measurement conditions, what minimum concentration level can we reliably observe in an image?
- Predicting visibility has two parts:
  1. We need to have appropriate x-ray counts for the compositional object and the background material. While experimental values can be used, in general such values will not be available, so we must simulate the spectrum. An EDS spectrum simulator such as NIST DTSA (Fiori, Myklebust, and Swyt) for the Macintosh platform or Nicholas Ritchie’s “Son of DTSA” for the pc platform can be used.

For DTSA:
NIST Desktop Spectrum Analyzer: Spectrum Simulator
The Basis for the Generated X-ray intensity

\[ I_{\text{gen}} = (\omega \ N_A \ \rho \ C_i / A) \ R \int_{E_c}^{E_0} \left( \frac{Q}{(dE/ds)} \right) dE \]

\( \omega = \) fluorescence yield \hspace{2cm} \( N_A = \) Avogadro’s number
\( \rho = \) density \hspace{2cm} \( C_i = \) mass concentration of i
\( A = \) atomic weight \hspace{2cm} \( R = \) backscatter loss
\( Q = \) ionization cross section
\( dE/ds = \) rate of energy loss
\( E_0 = \) incident beam energy \hspace{2cm} \( E_c = \) excitation energy

At each photon energy, calculate the specimen absorption:

\[ I_{\text{measured}} = I_{\text{generated}} \times f(\chi) \times \varepsilon \]

\( f(\chi) = \) absorption over depth distribution, x-ray fraction emitted
\( \varepsilon = \) detector efficiency
DTSA Spectrum Simulator:
Spectra of NIST SRM Glass K411 at Various Stages

NIST Glass K411
$E_0 = 20 \text{keV}$

As-generated

1. After specimen absorption
2. After EDS window absorption
3. After EDS broadening

Photon Energy (keV)
DTSA Spectrum Simulator: Measured and Simulated Spectra of NIST SRM Glass K411

Experimental DTSA Calculated

NIST Glass K411
$E_0 = 20\text{keV}$
Desktop Spectrum Analyzer (DTSA) Simulation

1 ms pixel dwell at 1MHz OCR

E<sub>0</sub> = 20 keV
0-20keV: ~1,000 counts

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<th>Element</th>
<th>Count</th>
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<td>O</td>
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<td>Na</td>
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• Predicting visibility has two parts:
  1. EDS spectrum predictor is needed, e.g., NIST DTSA. This estimates peak and background counts for putative objects.
  2. The x-ray image visibility predictor is based upon previous SEM image visibility research tools developed by David Bright (ref). With the counts predicted with DTSA for the characteristic peaks and continuum backgrounds, the Lispix image simulation tool constructs an image of objects with various shapes and sizes on a uniform background to create a template. Then apply Gaussian statistics appropriate to the count at each pixel to simulate image noise.

Step-by-step: (1) From “tools” menu, select “Xray Map Simulator”
Step-by-step: (2) To create a new image, under “File” select “New list”
Step-by-step: (3) A series of menus will appear; note that this series of menus will create a text file “New Object List” that can be saved under the main “File” menu with the “Save Text” command.
First task: give a specific name to the “New Object List” text file of instructions.
Step-by-step: (4) Choose image dimensions (default 300 x 200)
Step-by-step: (5) Choose background counts (default 15)
Step-by-step: (6) Choose data type
Step-by-step: (7) Choose treatment of overlapping objects, addition or replacement. This will matter for overlapping objects if the intensity of a pixel in the overlap pixels really is a sum of the intensity from objects “A” and “B”, or alternatively the overlap pixel is defined entirely by the intensity of the overlaid object.
Step-by-step: First line of file is now complete; now populate list with objects
Step-by-step: (8) From “Object List” tab select “Add Sample Object – plain values”
Step-by-step: A list of choices for object shape will appear
Step-by-step: (9) Select “Box – filled rectangle” which adds a line to the List that will define a rectangle with sides of 20 and 5 pixels located at Position 100 100 tilted 25 degrees from horizontal with intensity 40
Step-by-step: (10) To see the object specified by these instructions, under “Object List” choose “Make Map” which will produce the image shown giving the template of the map as full white on a black background.
Step-by-step: (11) To see the object with appropriate noise due to counting statistics, under “Map” choose “Add noise” which will produce the image shown next to the template.
Step-by-step: (12) To add another object, under “Object List” select “Add Sample Object – plain values”. This time a disc will be chosen centered at 200 150 with a radius of 20 and intensity 25.
Step-by-step: (13) To see the new template, under “Object List” select “Make Map” and then under Map” select “Add noise” to see final image.
Step-by-step: (14) To make a random collection of objects, after creating a new list, under “Object List” choose “Add Random Objects”
Step-by-step: (15) To make a random collection of objects, after creating a new list, under “Object List” choose “Add Random Objects”. A dialogue box will open allowing your choice of discs or boxes.
Step-by-step: (16) Next, a dialogue box will open allowing your choice of the number of objects (default = 5). We have chosen 9 for this example.
Step-by-step: (17) Next, a dialogue box will open allowing your choice of the size of the objects, e.g., for discs, the range of radii expressed as a percentage of the field width (default = 2% to 10%).
Step-by-step: (18) Next, a dialogue box will open allowing your choice of the intensity range relative to the background for the objects, e.g., (default = 70% to 200%).
Step-by-step: (19) The list of random objects will be written. If any of them intersect the boundary of the frame, a warning message will appear.
Step-by-step: (20) To see the results, under “Object List” choose “Make Map” and under “Map” choose “Add Noise”.

Template

Noisy image