

# 3D Surface Reconstruction from SEM/BSE multi-detector images

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August 2023 - Dec 2024

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## 1. Overview

This script reconstructs 3D surfaces from SEM images obtained from at least 3 BSE detectors without prior knowledge of their orientation. The reconstruction is based on SVD decomposition, x and y gradient components are obtained using Radon transform, the full surface is reconstructed either by direct gradient integration or, preferably, by an FFT-based method by (Frankot et al., 1988). The whole strategy is based on the method described in (Neggers et al., 2021).

## 2. Method

Below we list the main steps of the method:

1. Load images  $I_i, i \in [1, N]$  with  $N \geq 3$  (see fig. 1)
  - It is supposed that the SEM image has information block (FOV, magnification, etc.) in the bottom side of the image. This block is automatically trimmed. If it is not the case, the user can manually trim the image.
  - Image names with the full path is stored in the log file.
  - If requested, a Gaussian filter is applied to the images.
2. A correlation matrix  $C_{ij}$  is constructed from the images  $I_i$  with components  $C_{ij} = \sum_{x,y} I_i(x,y)I_j(x,y)$ .
3. A Singular Value Decomposition (SVD) of the correlation matrix is performed:  $C_{ij} = \sum_{k=1}^N U_{ik}S_kV_{jk}$ .

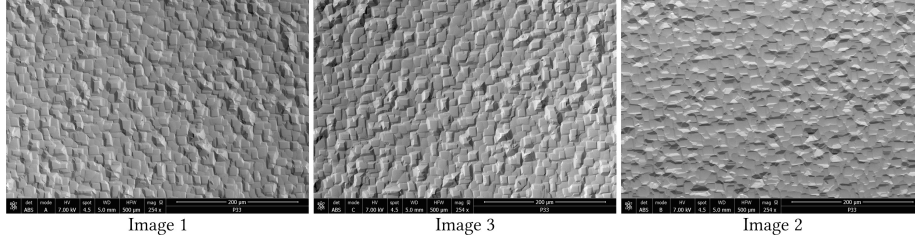


Figure 1: Original SEM images from three BSE detectors

4. The first three columns of the matrix  $U$  are used to construct the intensity image and two components of the gradient (along unknown principal directions) as follows (see fig. 2):

- Intensity:  $A = \sum_i U_{i1} I_i$ .
- Gradient 1:  $G_1 = \sum_i U_{i2} I_i / A$
- Gradient 2:  $G_2 = \sum_i U_{i3} I_i / A$

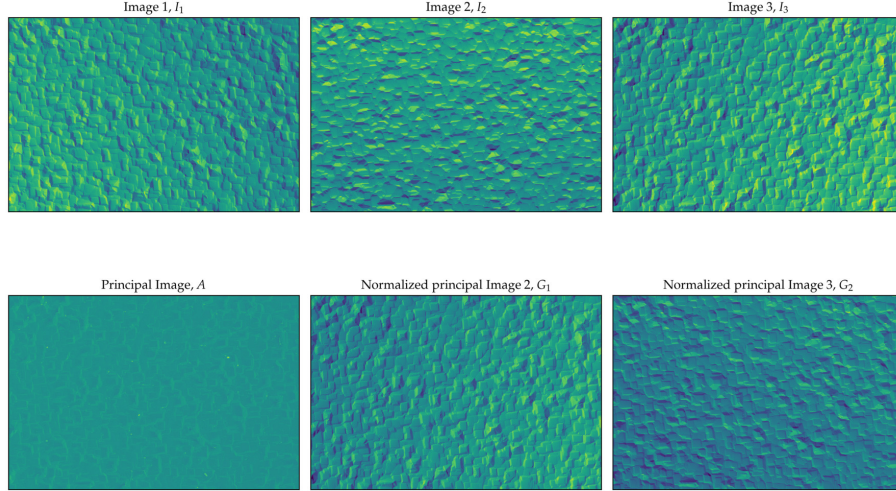


Figure 2: Original images  $I_1, I_2, I_3$  obtained with three detectors and their principal components  $A, G_1, G_2$  obtained through SVD

5. The  $x$  and  $y$  components of the gradient are obtained by using Radon transform of the gradient images  $G_1$  and  $G_2$ . Specifically, we keep only the circular region of  $G_1$  and null all data around (requirements of the Radon transform module). Then we compute Radon transform  $R(\theta)$  and

compute its RMS for every value of  $\theta$  (see fig. 3). Since Radon transform is computationally intensive, we apply it on  $G_1$  only and discretize probe  $\theta \in [0, \pi]$  in 180 points. The angle  $\theta_1$  corresponding to the minimum RMS is the angle of the first principal direction  $\theta_1$  (see fig. 3). The second principal direction  $\theta_2$  is perpendicular to the first one. It could be evaluated in the same manner using  $G_2$ .

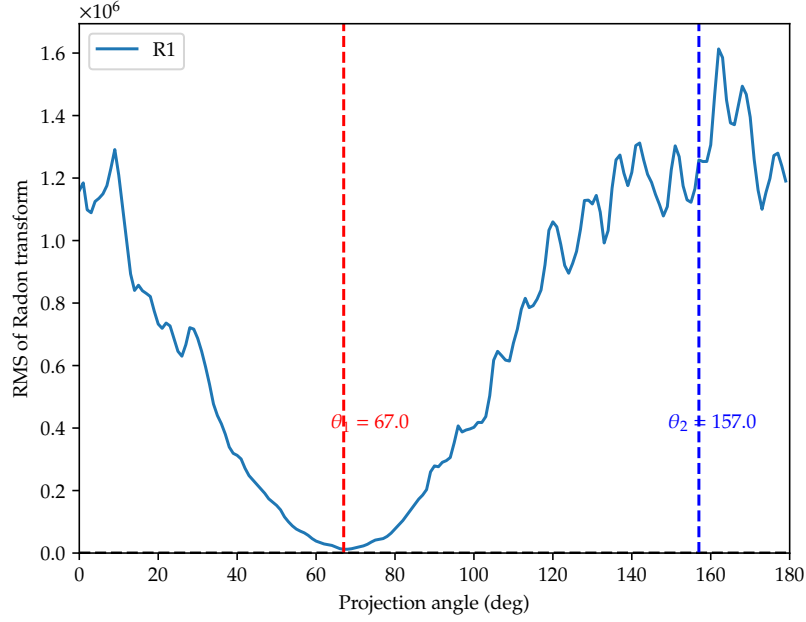


Figure 3: RMS of the Radon transform of the gradient image  $G_1$

6. The  $x$  and  $y$  components of the gradient are then obtained as follows:

- $G_x = G_1 \cos(\theta_1) + G_2 \cos(\theta_2)$
- $G_y = G_1 \sin(\theta_1) + G_2 \sin(\theta_2)$

In addition, a macroscopic tilt is subtracted from these gradients (see fig. 4). The tilt is computed as the average of the gradients over the whole image.

- $G_x = G_x - \langle G_x \rangle$
- $G_y = G_y - \langle G_y \rangle$

where  $\langle G_x \rangle$  and  $\langle G_y \rangle$  are the average values of the gradients  $G_x$  and  $G_y$ .

7. To reconstruct the surface from the gradients  $G_x = \partial z / \partial x$  and  $G_y = \partial z / \partial y$ , we use a method based on Fourier transform, see (Frankot et al., 1988). The Frankot & Chellappa method, providing very high reconstruction quality (see fig. 5), is based on the following Fourier transform pair:

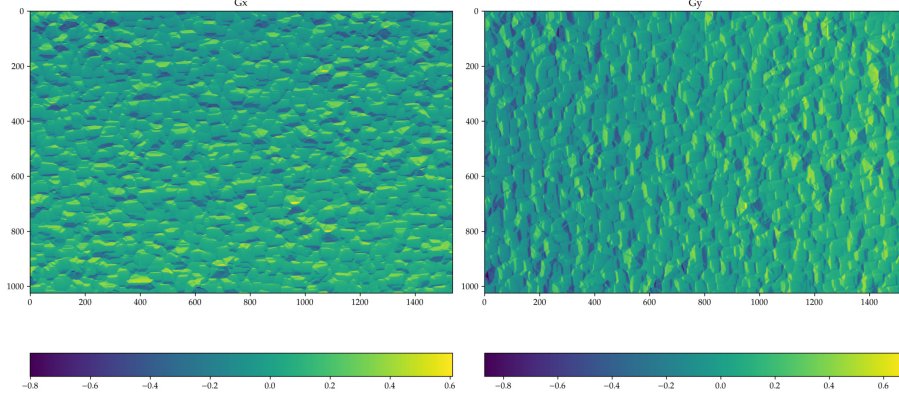


Figure 4: Gradients  $G_x = \partial z / \partial x$  and  $G_y = \partial z / \partial y$

- $\partial^2 z / \partial x^2 \leftrightarrow -k_x^2 \hat{z}(k_x, k_y)$
- $\partial^2 z / \partial y^2 \leftrightarrow -k_y^2 \hat{z}(k_x, k_y)$  where  $\hat{z}(k_x, k_y)$  is the Fourier transform of the surface  $z(x, y)$  and  $k_x, k_y$  are the wave numbers. The surface is then reconstructed as follows:
- $\hat{z}(k_x, k_y) = -\frac{1}{k_x^2 + k_y^2} (k_x \hat{G}_x(k_x, k_y) + k_y \hat{G}_y(k_x, k_y))$
- $z(x, y) = \mathcal{F}^{-1} \{ \hat{z}(k_x, k_y) \}$  where  $\mathcal{F}^{-1}$  is the inverse Fourier transform and  $\hat{G}_x(k_x, k_y)$  and  $\hat{G}_y(k_x, k_y)$  are the Fourier transforms of the gradients  $G_x$  and  $G_y$ .

If one wants to reconstruct main features of the roughness and ignore or smooth out small scale roughness, then a cut-off frequency can be introduced, in the GUI it is called **FFT cutoff** and provides the maximal wave number  $k_{\max}$  (in percentage of Niquist frequency) beyond which the Fourier components are set to zero.

7.b. An alternative method is a direct integration along  $x$  and  $y$  direction followed by minimizing distance between adjacent profiles and averaging between profiles integrated along  $x$  and  $y$ . In general, this method provides results of much lower quality, and is based on the following relations: + Assume that the first profile along  $y$  is zero  $z_x^{1,j} = 0$  for  $j \in [1, N_y]$ . + Integrate the first profile along  $x$  direction  $z_x^{i+1,1} = z_x^{i,1} + G_x^{i,1} \Delta x$  for  $i \in [1, N_x - 1]$ , where  $\Delta x$  is the pixel size. + Integrate next profile along  $x$  direction  $\tilde{z}_x^{i+1,j} = z_x^{i,j} + G_x^{i,j} \Delta x$  for  $i \in [1, N_x - 1]$  and  $j \in [2, N_y]$  and remove the average difference with respect to the previous profile  $\tilde{z}_x^{i+1,j} = \tilde{z}_x^{i+1,j} - \langle \tilde{z}_x^{i+1,j} - z_x^{i+1,j-1} \rangle$ . + Repeat the previous step for all profiles along  $y$  direction using  $G_y$  to get  $z_y^{i,j}$ . + Remove the average value of  $z_x^{i,j}$  and  $z_y^{i,j}$ , i.e.  $\tilde{z}_x^{i,j} = z_x^{i,j} - \langle z_x^{i,j} \rangle$  and  $\tilde{z}_y^{i,j} = z_y^{i,j} - \langle z_y^{i,j} \rangle$ . + Construct

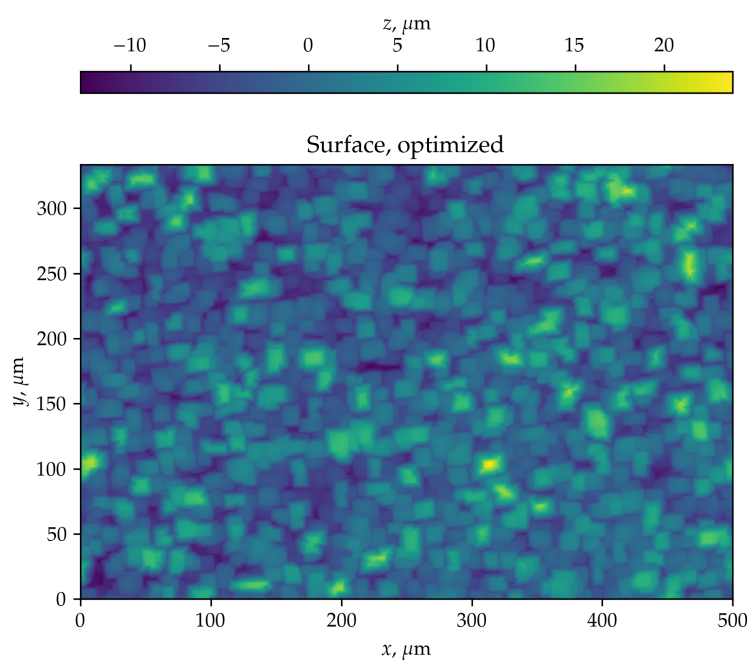


Figure 5: FFT reconstruction of the surface  $z(x, y)$

the final surface as  $z(x, y) = \frac{1}{2} (z_x^{i,j} + z_y^{i,j})$ .

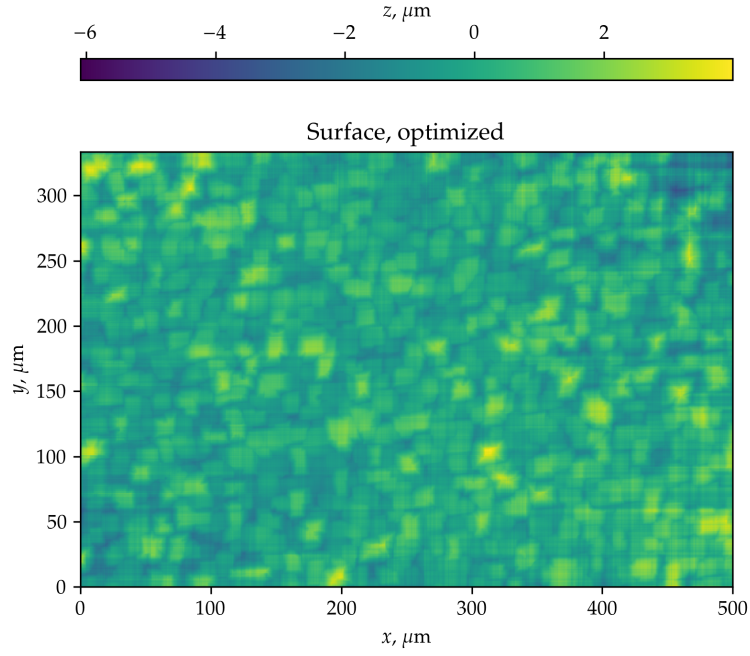


Figure 6: Reconstructed surface  $z(x, y)$  using direct integration

8. The final step is the removal of the curvature of the surface. This is done by fitting a parabolic surface in principal axes

$$z(x, y) = \frac{x^2}{R_x^2} + \frac{y^2}{R_y^2} + z_0$$

and subtracting it from the surface. The curvatures  $R_x, R_y$  and the off-set  $z_0$  are obtained by the least square fitting procedure.

## References

- Frankot, R. T. and Chellappa, R., A Method for Enforcing Integrability in Shape from Shading Algorithms, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. **10**, no. 4, pp. 439–51, 1988.
- Neggers, J., Hérupré, E., Bonnet, M., Boivin, D., Tanguy, A., Hallais, S., Gaslain, F., Rouesne, E. and Roux, S., Principal Image Decomposition for Multi-Detector Backscatter Electron Topography Reconstruction, *Ultramicroscopy*, vol. **227**, p. 113200, 2021.