

## STEM SI Warp: a Digital Micrograph script tool for warping the image distortions of atomically resolved spectrum image

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Besides conventional imaging techniques, an important capability of modern scanning transmission electron microscopy (STEM) is its integration with microanalysis techniques, such as electron energy loss spectroscopy (EELS) and energy dispersive X-ray spectroscopy (EDXS). In these methods, a focused electron probe raster across the sample and at each probe position imaging signal (s) (ADF or HAADF) and analytical signal(s) can be acquired simultaneously. The marked progress of the instrumentation hardware, i.e., aberration correctors, monochromators, better detectors /cameras, and more stable electron optics, sample holder and instrument environments, has made the chemical analysis at atomic resolution readily possible nowadays. Generally, STEM EELS and EDXS require much higher electron dose and longer dwell time (pixel exposure time) than STEM imaging. As a consequence, the scanning distortion becomes more serious in spectrum imaging. In case of lower-magnification spectrum mapping, these instabilities may be negligible, but at atomic resolution level, instabilities combined with long dwell times may create substantial image distortions, i.e. expansion, compression, and/or shearing of the lattice, that limit the interpretability of the spectrum image.

In this contribution, we report the development of a software tool, written in Digital Micrograph scripting language [1, 2], to post correct the image distortions of atomically resolved spectrum images. It can be used to correct two typical image distortions, i.e., linear (Fig. 1a) and nonlinear (Fig. 1b) distortions, as shown in Fig. 1. Two methods have been implemented to correct these distortions, pure pixel shift (i) without and (ii) with bilinear interpolation. Bilinear interpolation [3] considers the closest 2x2 neighborhood of known pixel values surrounding the unknown pixel. It then takes a weighted average of these 4 pixels to arrive at its final interpolated value. The weight on each of the 4 pixel values is based on the computed pixel's distance from each of the known points. With the prior knowledge of the crystal structure, the diagnosis of the image distortions was performed on the simultaneously acquired ADF. Then, the correction of image distortions was applied to ADF, SI and/or elemental maps. Using two practical examples, i.e., 2-dimensional Ba doped  $\text{La}_2\text{CuO}_4$  [4, 5] and  $\text{SrTiO}_3$  bulk material, we demonstrate that the script could correct the image distortions and warp the deformed SI, finally resulting in a refined color elemental map.

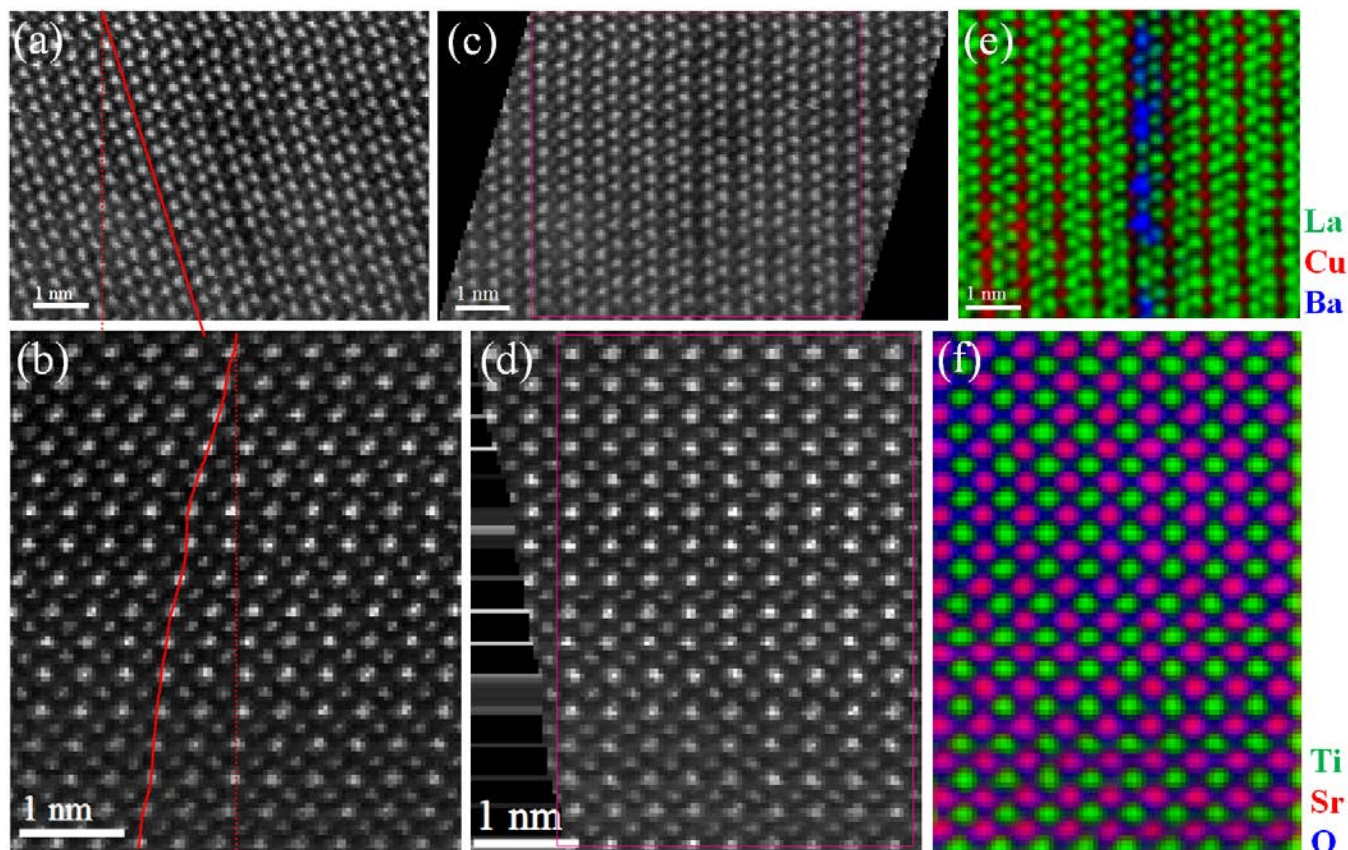
The plugin was composited by several scripts: scripts for linear and nonlinear warping, scripts for synchronizing the ROI between the images and for cropping the ROI as new image, and a script for filtering the final color map. This plugin is available by request to the authors [6].

### References:

- [1] B Schaffer in "Transmission Electron Microscopy, Diffraction, Imaging, and Spectrometry" ed. C.B. Carter and D.B. Williams, (Springer, Switzerland), Chapter 6, p.167.
- [2] D R G Mitchell, B Schaffer, *Ultramicroscopy* **103** (2005), p.319.
- [3] [https://en.wikipedia.org/wiki/Bilinear\\_interpolation](https://en.wikipedia.org/wiki/Bilinear_interpolation) [Accessed 24January2017]
- [4] Y Wang *et al.*, *ACS Appl.Mater.Interfaces* **8** (2016), p.6763.

[5] F Baiutti *et al.*, ACS Appl.Mater.Interfaces **8** (2016), p.27368.

[6] The research leading to these results has received funding from the European Union Seventh Framework Program under Grant Agreement 312483-ESTEEM2 (Integrated Infrastructure Initiative I3).



**Figure 1.** Typical image distortions in spectrum imaging: (a) linear and (b) nonlinear distortions. As can be seen the straight lattice (indicated by the dotted lines) has been distorted into an inclined or curved line. (c) Linear image distortion removed ADF image, the raw ADF image is shown in Fig. a. (d) Nonlinear image distortion removed image, the raw ADF image is shown in Fig. b. (e) Final warped and cropped RGB color figure of the Overlaid elemental maps, Cu-L<sub>2,3</sub>(Red), La-M<sub>4,5</sub> (Green), and Ba-M<sub>4,5</sub> (Blue). (f) Final warped and cropped RGB color figure of the overlaid elemental maps, Sr-L<sub>2,3</sub> (Red), Ti-L<sub>2,3</sub> (Green), and O-K (Blue). The STEM-EELS experiments were performed on a JEOL JEM-ARM 200CF microscope with Gatan GIF Quantum ERS electron energy-loss spectrometer operated at 200kV. A collection semi-angle of 111 mrad and 5 ms dwell time were used for the EELS acquisition. The SIs was de-noised by the multivariate weighted principal component analysis.