Strain Mapping in HRTEM Images

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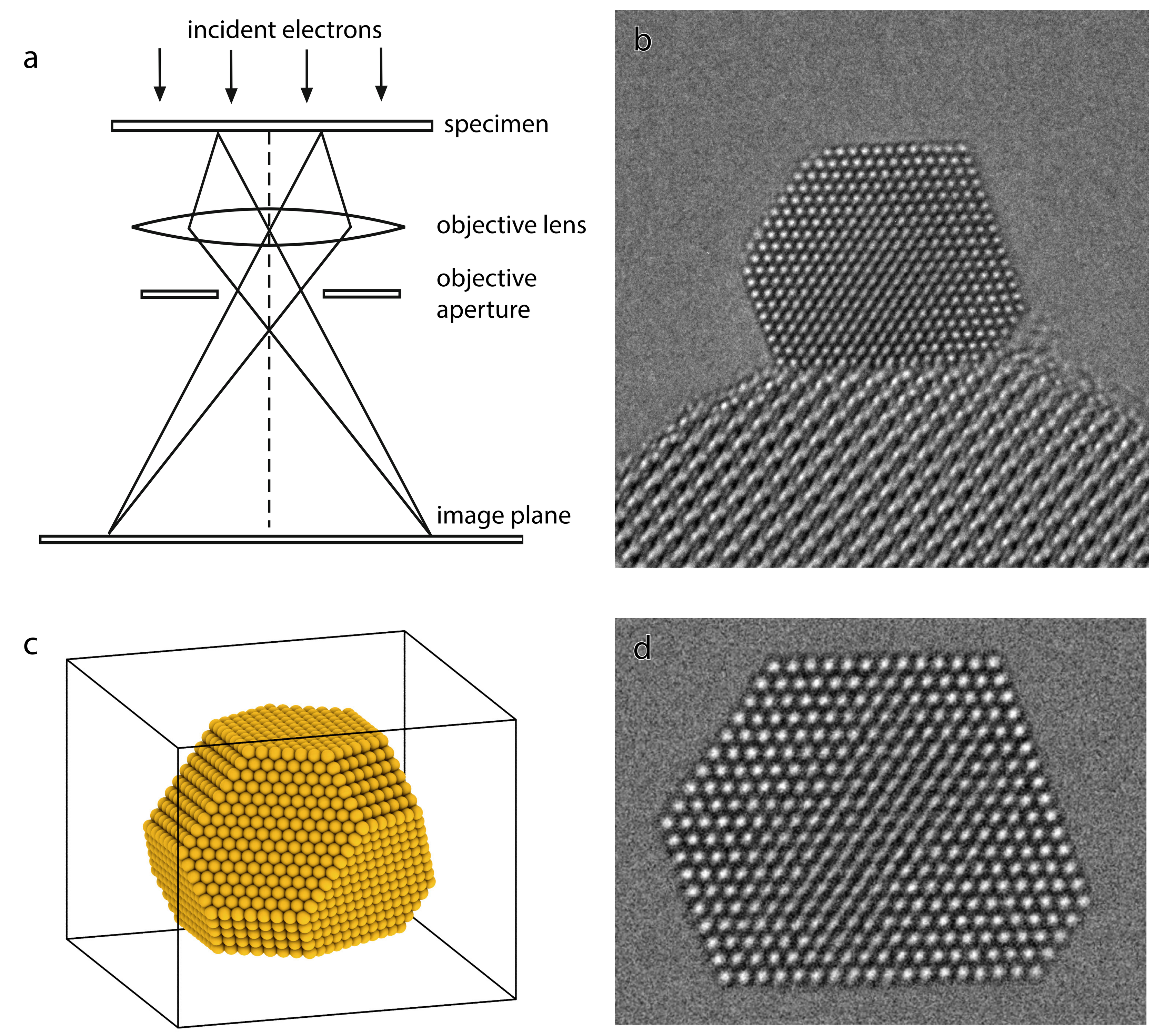
Simulated HRTEM Images

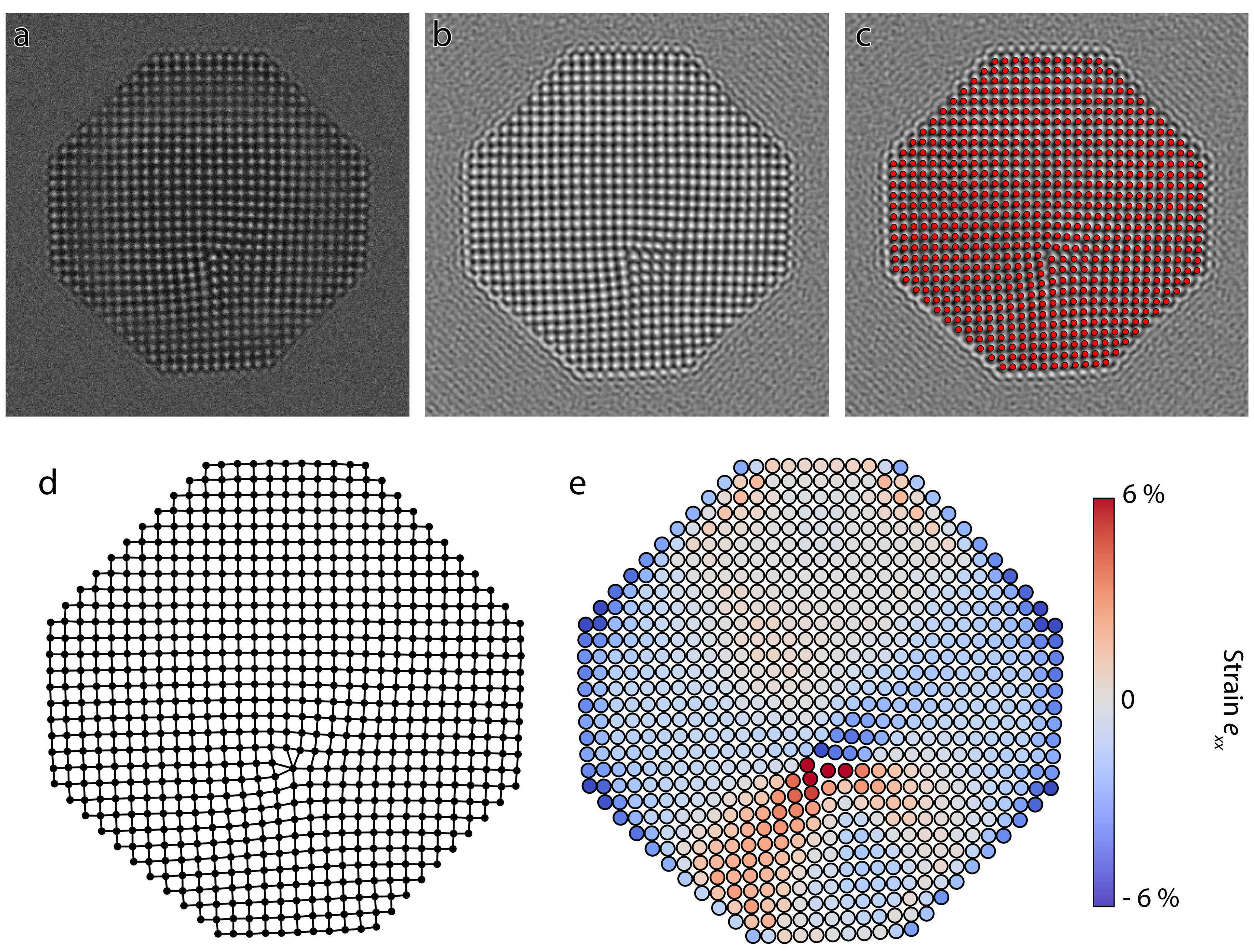
High-resolution transmission electron microscopy is capable of resolving the structure of nanoparticles down to the position of individual atomic columns. Simulated images provides a convenient tool to improve and benchmark image analysis procedures. This is particularly important due to image abberations caused by for an example defocus and crystal tilt.



(a) The optics of a typical transmission electron microscope. (b) An experimental HRTEM image of a gold nanoparticle supported on cerium oxide. (c) The possible three-dimensional structure of the nanoparticle. (d) A simulated HRTEM image. The image have been created to match the nanoparticle in the experimental image as closely as possible.

Strain Mapping

Important information about defects, surface and interfacial structure are hidden in the positions of atomic columns, a map of the distribution of local elastic strain is useful to reveal this information.



(a) Original noisy image. (b) The correlation coefficient of the image with a peak template . (c) The peaks are chosen based on their local relative intensity. (d) Lattice generated by relating the local environment of each peak to a template. (e) A map of the strain clearly highlighting a dislocation, as well as the relaxation of the surface.

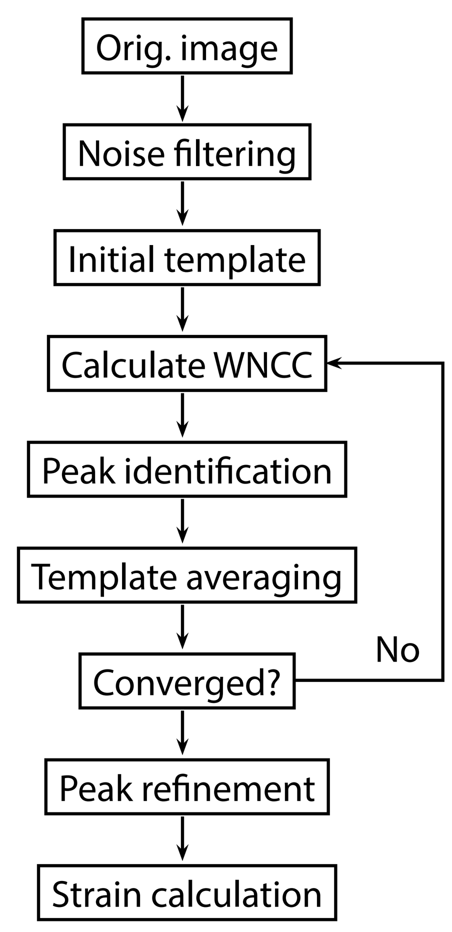
Algorithm in Detail

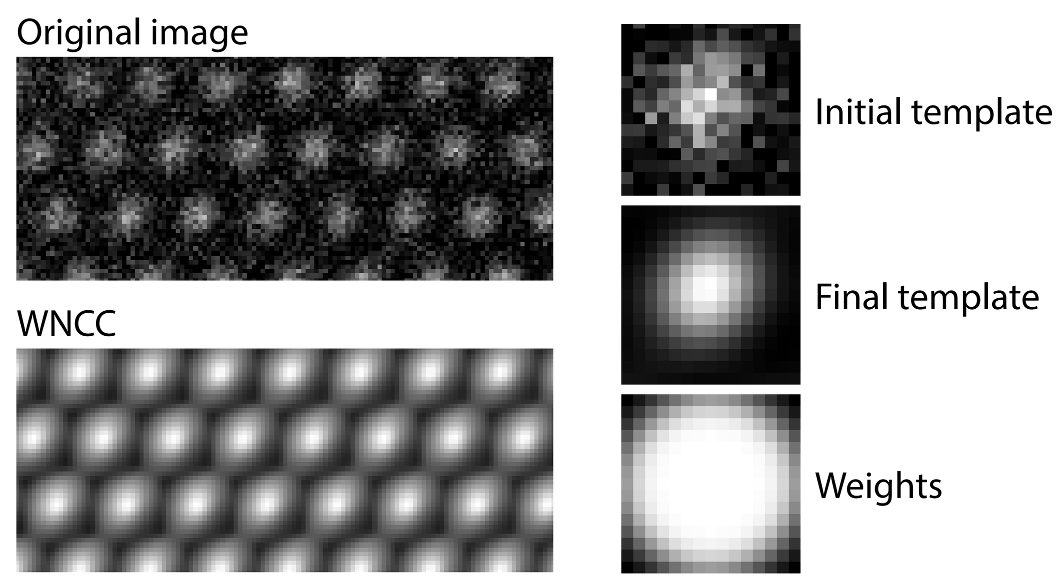
The template for the correlation coefficient is optimized in a loop. New iterations of the template are created by averaging regions around each peak, as the template improves more peaks are correctly identified. The loop is terminated when the identified peaks are identical.

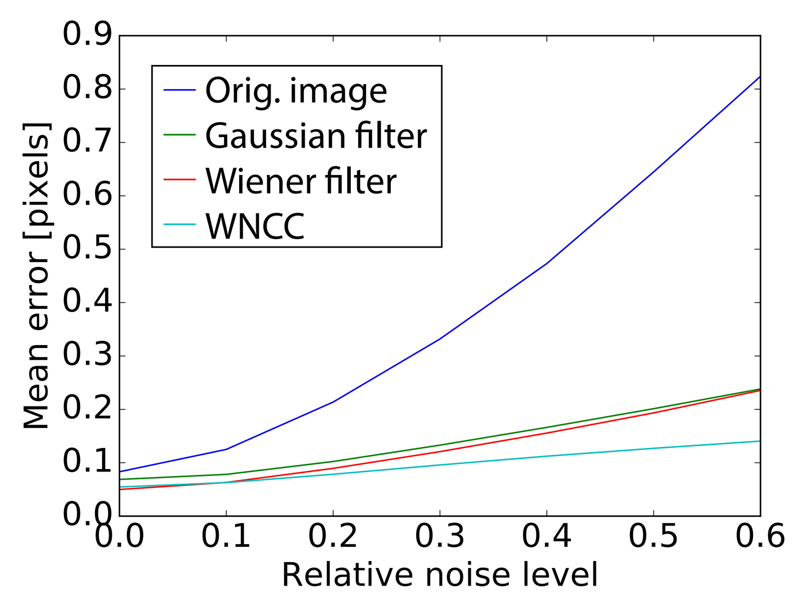
Weighted normalized correlation coefficient

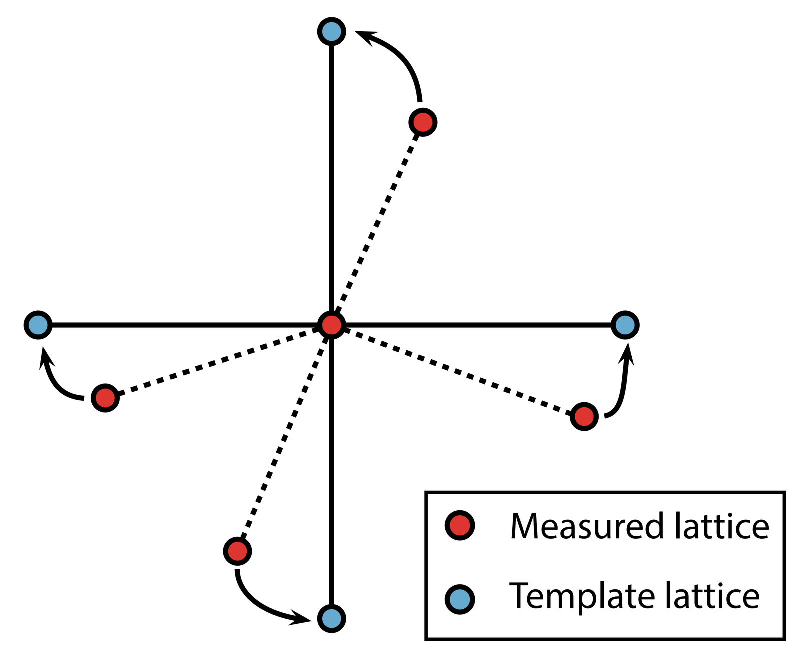
$$\mathrm{WNCC}(X,Y,W)=\frac{\sum_i W_i(X_i-\bar{X})(Y_i-\bar{Y})}{\sqrt{\sum_i W_i(X_i-\bar{X})}\sqrt{\sum_i W_i(Y_i-\bar{Y})}}$$

where $X,\ Y,\ W$ are vectors representing the image, template and weights respectively.







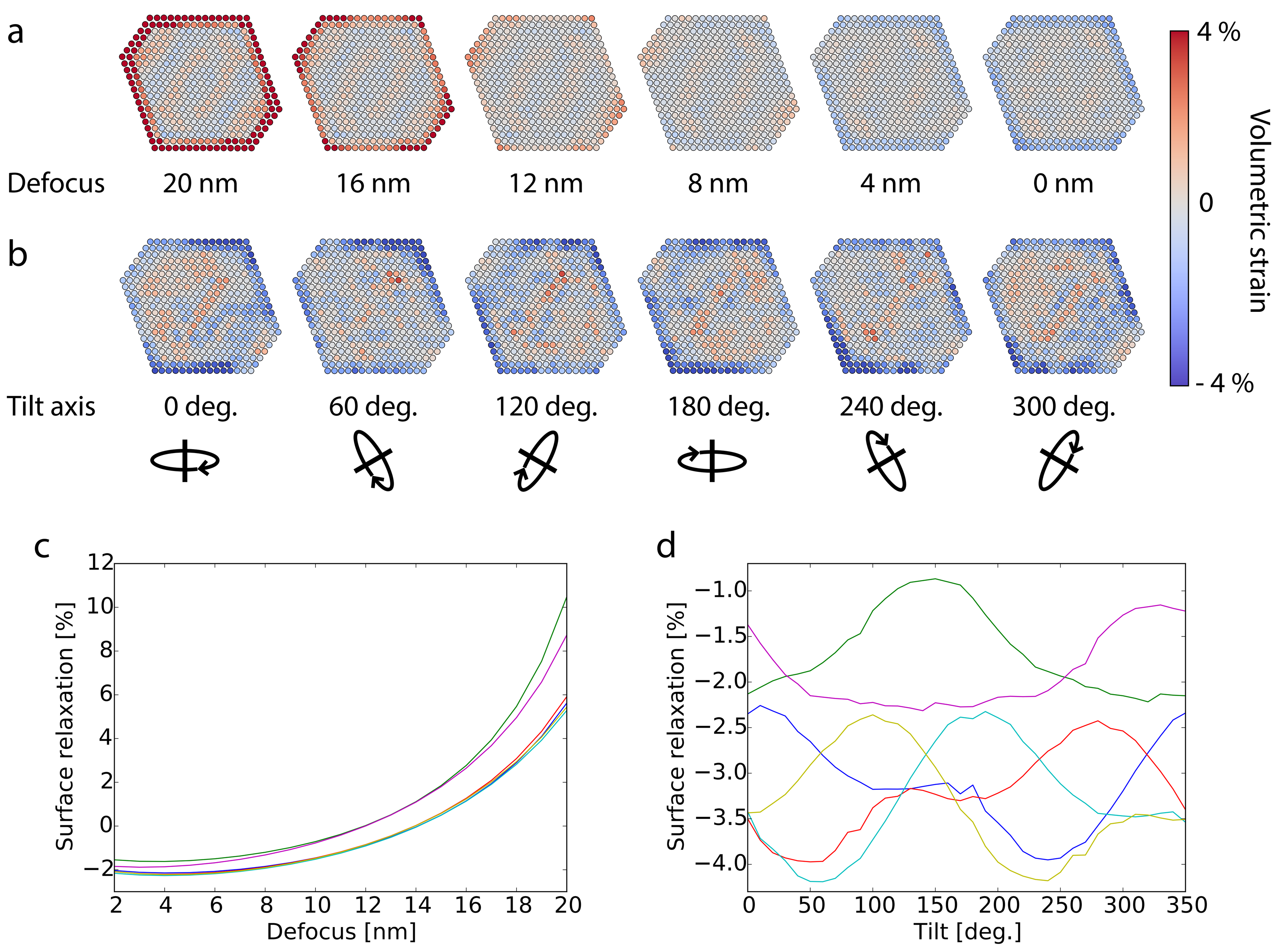


The mean error measured as the distance between the real and measured peak position. A comparisson is made between commonly used filters and the algorithm based on the WNCC.

The optimal affine transformation between the measured and ideal local lattice is found. The lattice orientation and strain is obtained from a left-sided polar decomposition $PU = A$.

Influence of Abberations

The measured strain map is affected significantly by optical abberations, the most prominent of these are defocus and tilt.



(a) Series of strain maps with varying defocus. (b) Series of strain maps of a slightly tilted nanoparticle with varying tilt axis. (c) Surface relaxations measured for varying defocus, each line corresponds to a different facet of the nanoparticle. (d) Surface relaxations measured for varying tilt axis.

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