**The maximum a posteriori probability rule to detect single atoms from low signal-to-noise ratio scanning transmission electron microscopy images**

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Single atom detection is of key importance to solve a wide range of scientific and technological problems. Scanning transmission electron microscopy (STEM) is a powerful technique to image single atoms. However, to overcome beam damage, the incoming electron dose should be kept low enough resulting into images exhibiting a very low signal-to-noise ratio (SNR) and extremely weak contrast especially for light-element nanomaterials. In general, visual inspection of such images leads to biased structure information. To overcome this problem, the maximum a posteriori (MAP) probability rule is proposed enabling one to detect single atoms with high reliability.

The validity and usefulness of the MAP probability rule has been demonstrated to experimental and simulated ADF STEM images of samples of arbitrary shape, size and atom type. First, an experimental low SNR high-angle annular dark-field (HAADF) image of a material with known structure, $SrTiO_3$ (figure 1(a)), has been analysed. The most probable structure indicated by the MAP probability rule is shown in figure 1(b), corresponding to the expected crystal structure in [100] direction. Next, the MAP probability rule has been applied to detect the individual atoms near the edge of a Au nanorod from an experimental HAADF STEM image (figure 1(c)) (Van Aert et al., 2013). The most probable structure is shown in figure 1(d). Moreover, to test its limits, the same approach has been applied to a simulated HAADF image with lower incoming electron dose (figure 1(e)). Only one extra atom has been detected by the MAP probability rule where the simulation did not include an atom. This atom is indicated by the arrow in figure 1(f). Finally, the most probable structure from an experimental HAADF image of a Ge cluster (figure 1(g)) (Bals et al., 2012) is shown in figure 1(h) providing more accurate results than what can be obtained from visual inspection of such an image.

In conclusion, the MAP probability rule has been introduced to detect single atoms from low SNR STEM images. By combining parameter estimation and model-order selection, the most probable atomic structure of unknown nanomaterials can be determined in an automatic and objective manner. This information is of great importance for the analysis of radiation sensitive and light-element nanostructures, where visual inspection of images may lead to biased results.

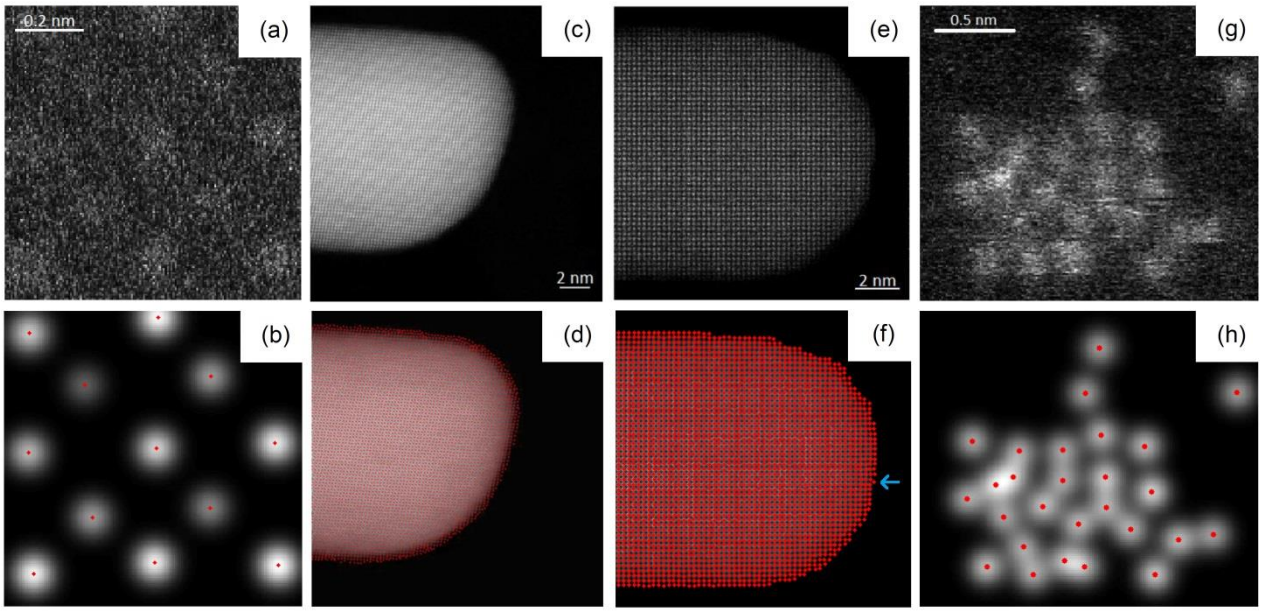

Figure 1: (a) Experimental HAADF image of $SrTiO_3$ [100] with an incoming electron dose of (1.08 ± 0.05)·$10^4$ $e^-/Å^2$. (c) Experimental HAADF image of a Au nanorod with an incoming electron dose of around 2·$10^5$ $e^-/Å^2$. (e) Simulated HAADF image of a Au nanorod with an incoming electron dose of 5000 $e^-/Å^2$ and source size broadening with a FWHM of 0.7 Å. (g) Experimental HAADF image of a Ge cluster with an incoming electron dose of around 6.8·$10^4$ $e^-/Å^2$. (b), (d), (f), (h) Most probable parametric models from the experimental data in (a), (c), (e) and (g), respectively, indicated by the MAP probability rule with the detected atom columns shown in red.

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