A journey from order to chaos — Atom by atom transformation from graphene to a 2D carbon glass

Supplementary Information

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Abstract

This supplementary information contains an example of the method used for obtaining the atomic structures from the TEM images, as well as images of all obtained structures and descriptions for additional supplementary material.

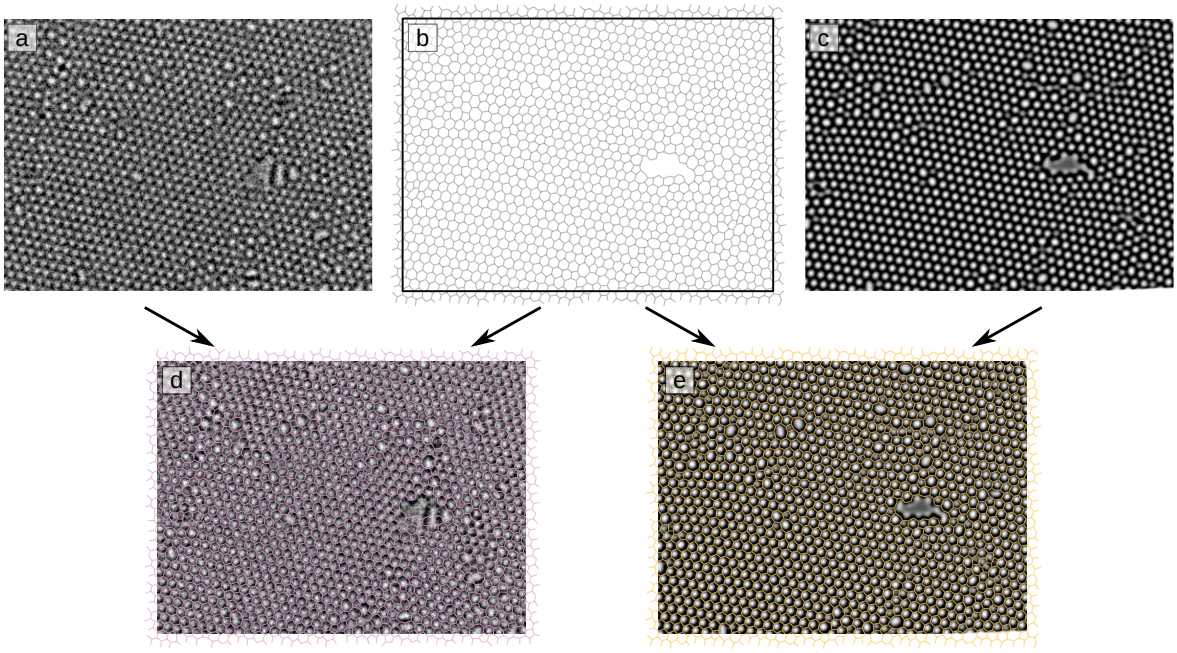

Figure S1: **Comparison of the extracted atomic structure and the original TEM image.** (a) A high dose TEM image (for higher signal-to-noise ratio, 4 images have been averaged). (b) Atomic structure extracted from the TEM image. (c) Simulated TEM image based on the model structure. (d, e) The real and simulated TEM images with an overlay of the respective structure (panel b).

Obtaining the atomic structure from TEM images

The atomic coordinates have been extracted from TEM images as described in the original article. An example of a high irradiation dose case is shown in Fig. S1. We extracted the structure (Fig. S1b) from the TEM image of Fig. S1a, and used it as a basis for TEM image simulation [1] (Fig. S1c), to allow a direct comparison. Comparison of the real and simulated TEM images — with and without overlaid atomic structure (see Fig. S1) — shows that nearly all carbon rings have been correctly interpreted by our method.

TEM images and derived atomic structures

In Figs. S2-S6, we provide all TEM images and the corresponding atomic structures, which were used in the analysis of shortest path ring statistics (Fig. 4a-f of the article).

Structures shown in Fig. S2a, Fig. S5a and Fig. S6b were further used for the structure analysis (Fig. 2 of the article), and the structures as presented in Fig. S4a and S5a were the basis for the analysis of the intermediate-range order (radial and angular distribution functions) presented in Fig. 3 of the article. Note that the weak ring-shaped features slightly left from the center in Fig. 1c of the main article and in Fig. S5c and S6 are a distortion from the CCD camera.

Description of additional supplementary material

In file `at_coords.zip`, we provide the xyz-coordinate files of the atomic structures illustrated in Figs. S2-S6. The filename is constructed as: `rel_stru_dose_densitydeficit.xyz` (the dose is given in units of 10^9 e^-/nm^2 and the density deficit in %). The format of the coordinate files is as follows: the first line contains the number of atoms, while the second line is a comment, and the rest of the file lists the atomic coordinates in the following order: atomic element, x-coordinate, y-coordinate and z-coordinate. All coordinates are given in Ångströms.

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[1] Koch, C. *Determination of core structure periodicity and point defect density along dislocations.* Ph.D. thesis (2002).

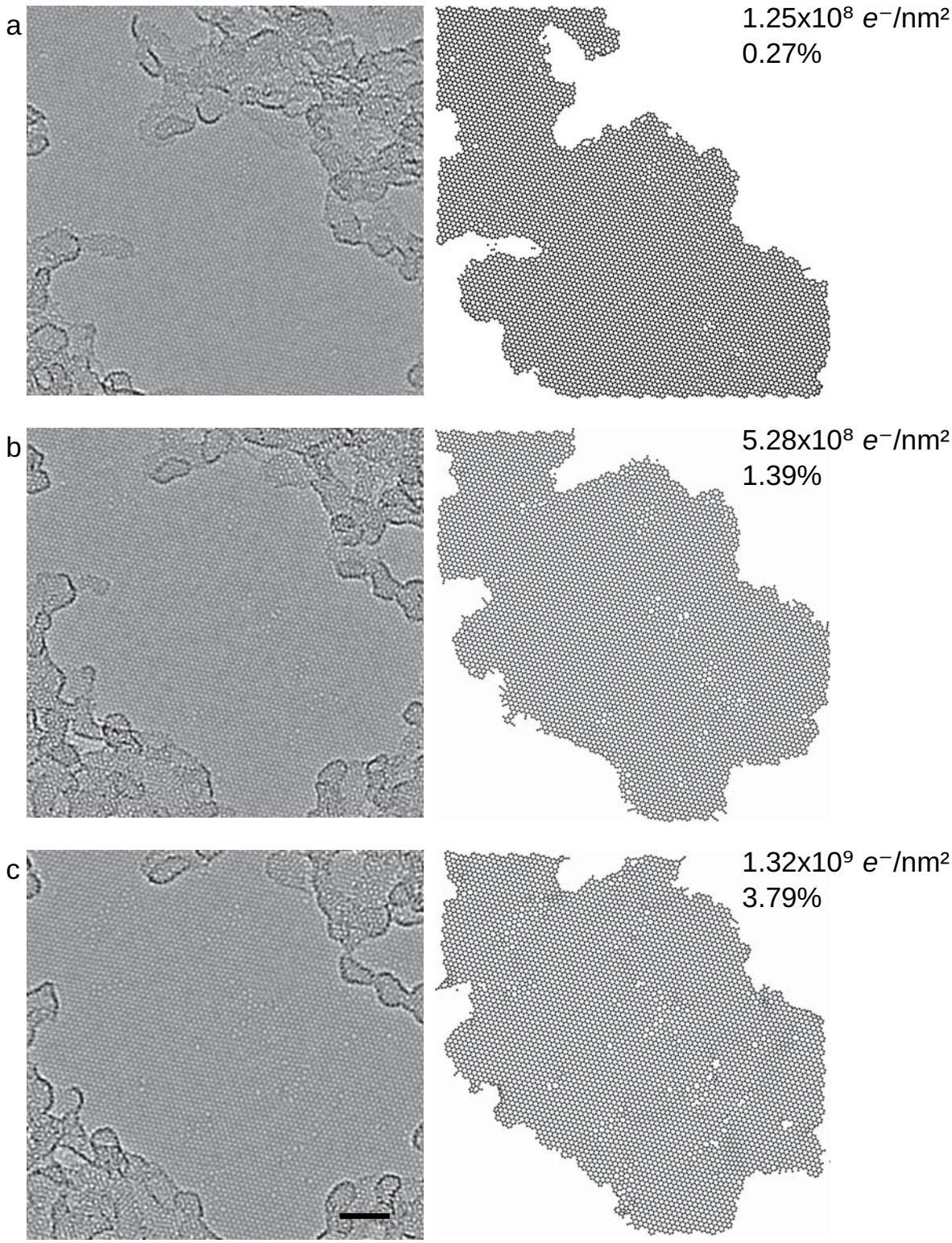

Figure S2: TEM images (left) and the corresponding atomic structures (right). The applied dose and the corresponding density deficit are given for each structure. Scale bar is 2.5 nm.

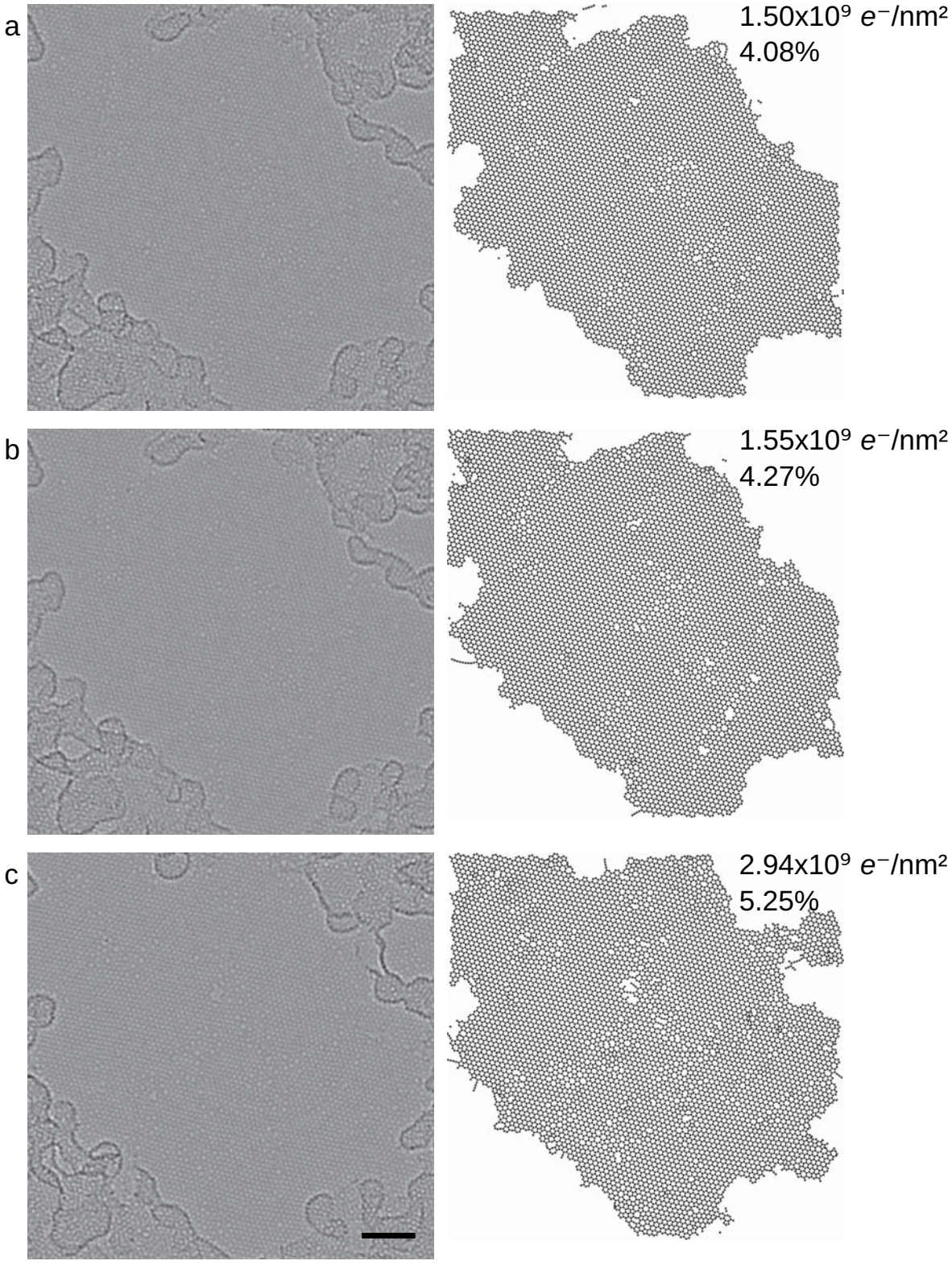

Figure S3: TEM images (left) and the corresponding atomic structures (right). The applied dose and the corresponding density deficit are given for each structure. Scale bar is 2.5 nm.

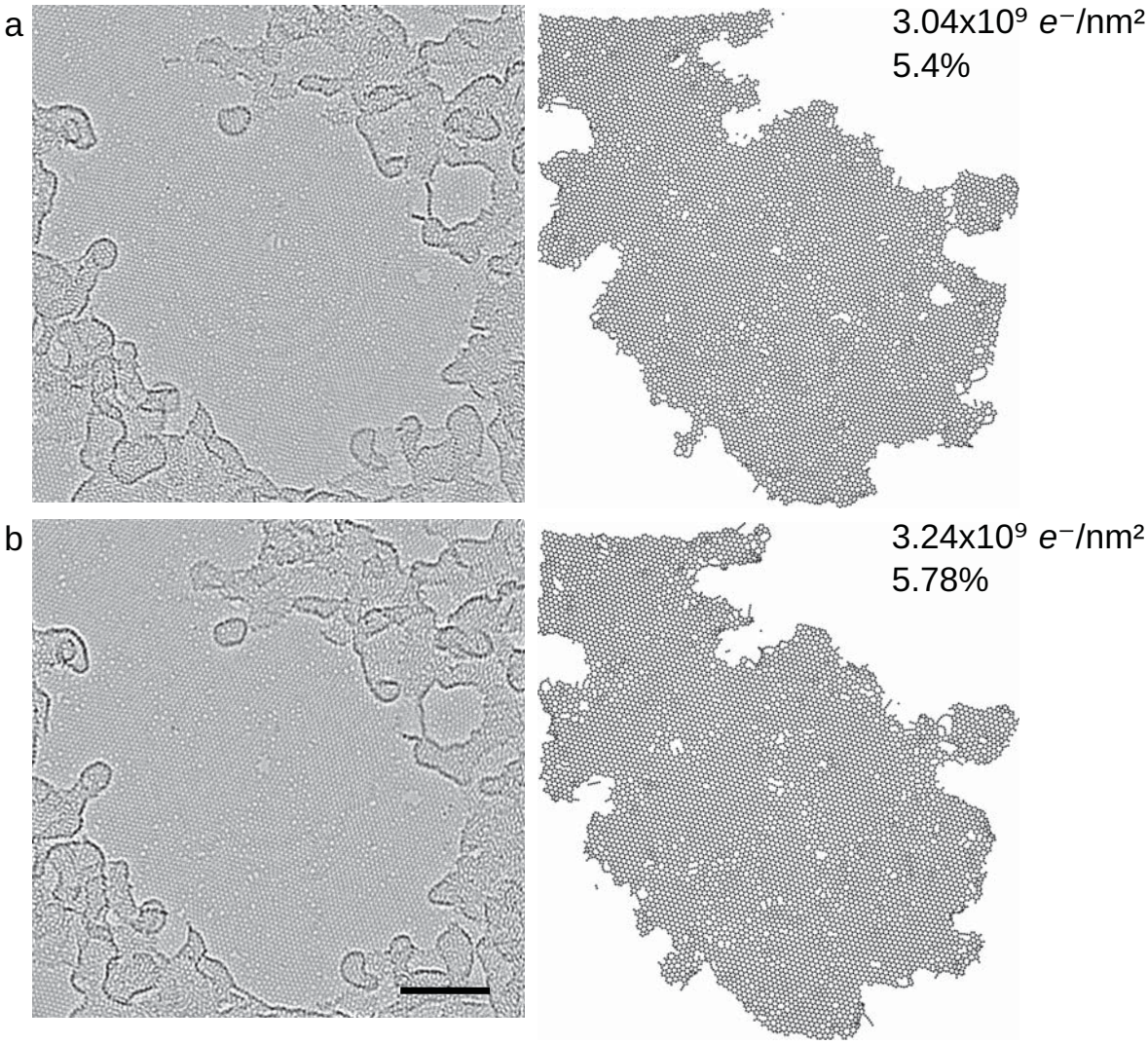

Figure S4: TEM images (left) and the corresponding atomic structures (right). The applied dose and the corresponding density deficit are given for each structure. Scale bar is 5 nm.

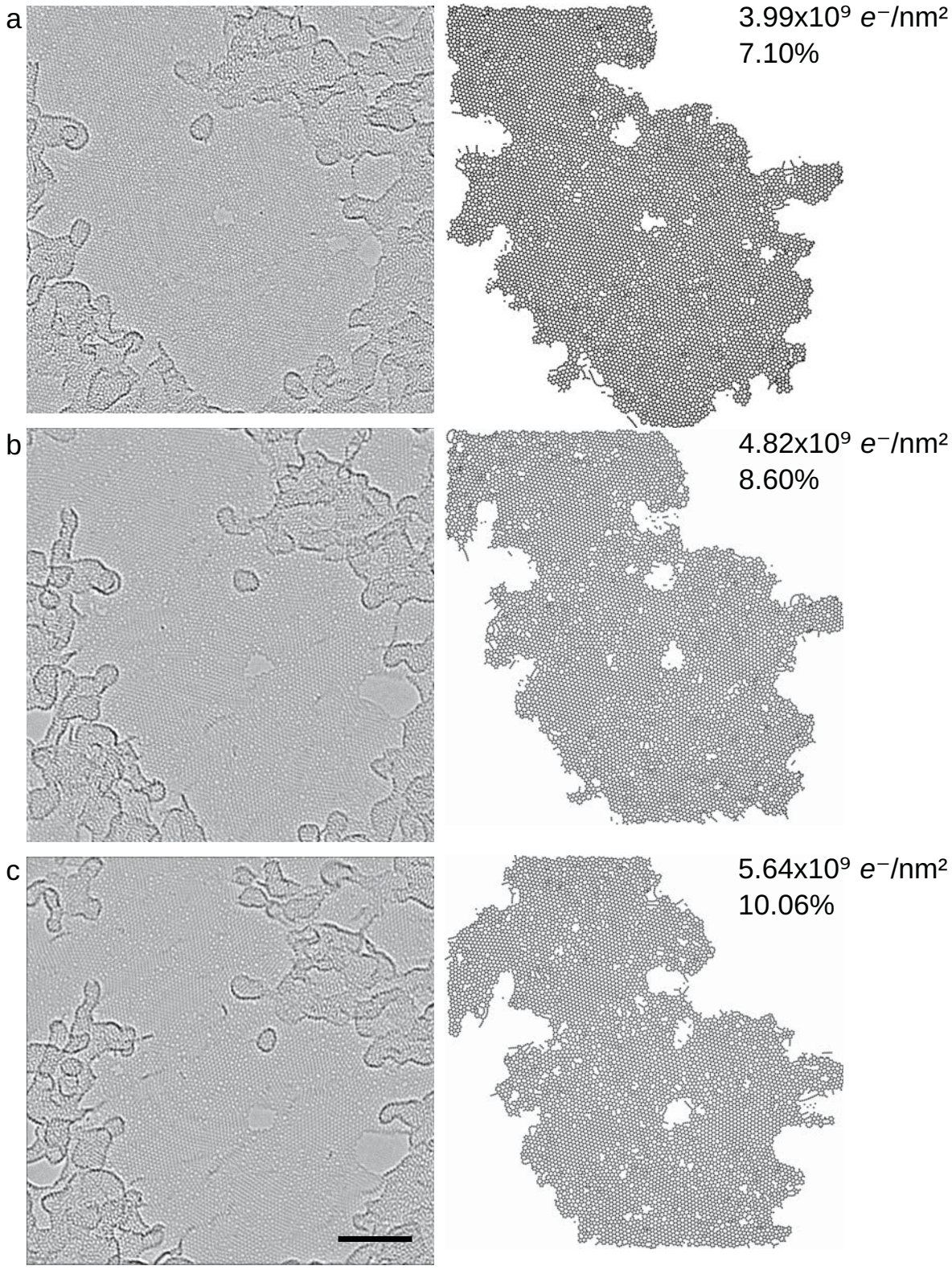

Figure S5: TEM images (left) and the corresponding atomic structures (right). The applied dose and the corresponding density deficit are given for each structure. Scale bar is 5 nm.

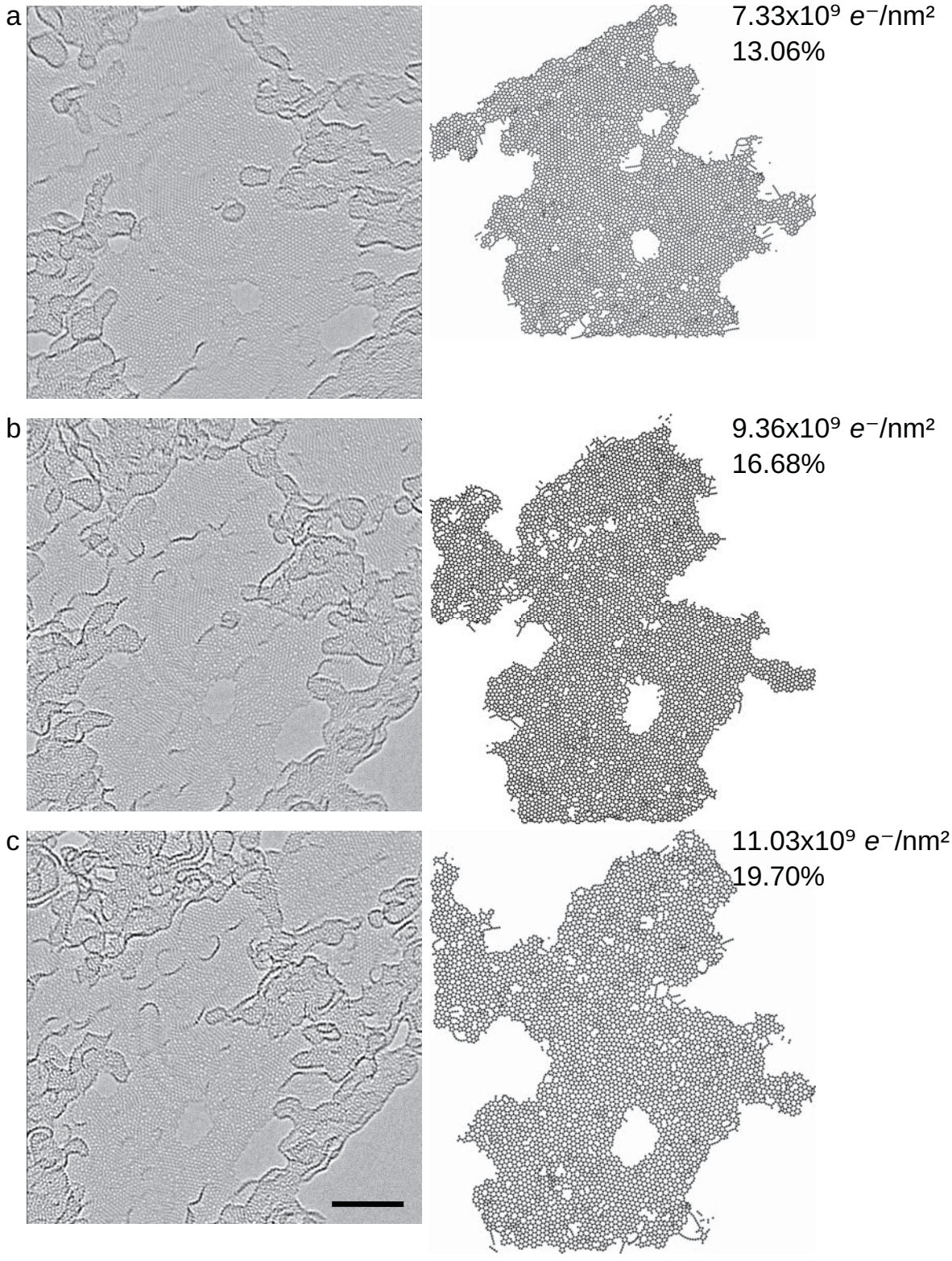

Figure S6: TEM images (left) and the corresponding atomic structures (right). The applied dose and the corresponding density deficit are given for each structure. Scale bar is 5 nm.