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Electron dose dependence of signal-to-noise ratio, atom contrast and resolution in transmission electron microscope images

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ABSTRACT

In order to achieve the highest resolution in aberration-corrected (AC) high-resolution transmission electron microscopy (HRTEM) images, high electron doses are required which only a few samples can withstand. In this paper we perform dose-dependent AC-HRTEM image calculations, and study the dependence of the signal-to-noise ratio, atom contrast and resolution on electron dose and sampling. We introduce dose-dependent contrast, which can be used to evaluate the visibility of objects under different dose conditions. Based on our calculations, we determine optimum samplings for high and low electron dose imaging conditions.

1. Introduction

The instrumental resolution of transmission electron microscopes (TEMs) has dramatically improved during the last decade, mainly due to the introduction and practical realisation of hardware aberration correction [1–3]. As a result, materials can now be imaged and identified down to single atomic columns [4,5] or, in the case of the new class of two-dimensional materials, even single atoms [6,7]. With the aim of reducing radiation damage induced by the imaging electrons, low-voltage aberration-corrected TEMs, down to voltages of 20 kV [8,9], 30 kV [10], and 40 kV [11], are currently under development. A voltage-tunable fully-corrected (that is, corrected for higher-order geometrical aberrations as well as chromatic aberrations of the imaging lenses [12]) TEM seems close to becoming reality [13].

Achieving the improved resolution of an aberration-corrected TEM requires, however, an infinite electron dose on the studied specimen, and only few materials can withstand very high, let alone infinite doses. Materials can be damaged via the knock-on damage mechanism, where atoms are displaced by direct impacts of the imaging electrons, and in such cases lowering of the electron energy below a material specific threshold is desirable [8,14–17]. On the other hand, the electron–electron (inelastic) scattering cross section increases at lower electron energies and, depending on the material, ionization can become the dominating damage mechanism [17]. Effective ways of reducing ionization damage may be cooling of the specimen [18] or conductive coating [19]. As extreme examples of the latter, samples have been enclosed within carbon nanotubes [9], or between graphene layers [20], greatly reducing radiation damage during imaging. Such approaches are not always feasible, however, and images thus need to be acquired with limited electron doses.

The stability of the microscope is another factor limiting the electron dose in a single image. The microscope tends to drift away from the corrected state, and as a result images can be acquired only within a small time window before resolution is deteriorated [21–23]. Also all kinds of instabilities including electrostatic and magnetic field noise [24] and instabilities caused by the sample stage can lead to blurring of the images, if long exposure times are used.

With all this in mind, microscopists have to develop strategies for limited electron dose imaging. Thus, having a robust framework for estimating the effects of this limitation is necessary. Here, we address this issue, by exploring the influence of the electron dose and sampling on the signal-to-noise ratio (SNR), the atom or lattice contrast, as well as the resolution, with the help of dose-dependent image simulations. We introduce a modified definition for the image contrast, which takes the electron dose into account. The dose related noise is treated as stochastic fluctuations around the ideal electron count at each image pixel, instead of the previously used additive noise [25–30]. Using these tools, we determine the optimal sampling for achieving atomic resolution images of graphene, as a function of the information limit and magnification of the microscope, as well as determine the required electron dose based on the calculated atom contrast. Graphene is used as the example material due to the simplicity of its structure, which allows straight forward interpretation of the results.

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2. Theoretical and experimental methods

2.1. Image simulation with finite electron dose

The structural information of the sample is carried primarily by elastically scattered electrons, which is distorted by an electromagnetic lens during the propagation process in the microscope. The distorted information is transferred to the detector and the average number of electrons collected by each detector pixel is determined by the electron dose, the sampling and the probability of the electron to be found on each pixel, which is the squared modulus of the image wave. The actual number of electrons collected by each detector pixel is governed by Poisson statistics.

In this paper we utilize the elastic model based on [31] in the image calculation for graphene at low voltages ranging from 20 kV to 80 kV on a C_s/C_c-corrected microscope. Inelastic scattering is not included for the following reason:

On a C_c-corrected microscope, the contrast delocalization caused by inelastic scattering in a single layer of graphene at voltages as low as 20 kV is negligible. In this case, the influence of inelastic scattering on the image is mainly the decrease of the intensity contributed by the elastic scattered electrons [32].Our image simulation with finite electron dose follows the order:

1. Generate the position distribution function. Obtain the probability distribution of the electrons by calculating the image intensity for the experimental imaging conditions with infinite dose. The experimental conditions include the accelerating voltage, aberration parameters, the size of the usable aperture determined by the aberration corrector and the damping functions. Since we search for the image conditions providing the maximum contrast, we determine the parameters giving the brightest atom contrast. The general procedure to search for the maximum contrast and the corresponding imaging conditions are presented in [31]. In addition, we include the influence of image spread E_{is}, focus spread E_{fs} and the MTF of the camera. For a phase object, the intensity I_i of the final image is a convolution between the calculated image I [31] and the damping functions:

$$I_i(\vec{\rho}) = \int \tilde{I}(\vec{q})E_{is}(\vec{q})E_{fs}(\vec{q})MTF(\vec{q})e^{i\vec{q}\vec{\rho}}\, d^2\vec{q}. \tag{1}$$

Image spread is caused by all kinds of noise causing a random deflection of the image. The origin of these zeroth-order aberrations is vibrations and drift of the stage, parasitic time-dependent fields resulting from instabilities of the lens currents and magnetic fields resulting from eddy currents in the material of the lenses as shown recently by Uhlemann et al. [24]. The combined effect of these disturbances on the image contrast is given by the envelope function [12]

$$E_{is}(\vec{q}) = \exp[-\tfrac{1}{2}(2\pi\sigma(C_\epsilon))^2 q^2]. \tag{2}$$

The spatial frequency $q = \theta/\lambda$ depends on the scattering angle θ and the wavelength λ of the electrons; $\sigma(C_\epsilon)$ denotes the standard deviation of the image spread.

The residual focus spread is caused by the movement of the stage and all the electromagnetic lenses in the z-direction and by the parasitic first-order aberrations of the focusing elements. The effect of the focus spread on the image contrast is expressed by the envelope function [12]

$$E_{fs}(\vec{q}) = \exp[-\tfrac{1}{2}(\pi\lambda\sigma(C_1))^2 q^4]. \tag{3}$$

Here $\sigma(C_1)$ denotes the standard deviation of the focus spread. In most cases, TEM images are recorded using charge-coupled detectors (CCD) with a fiber-optics coupled scintillator. In the ideal case, each electron is only detected by one of the detector pixels. The number of detected electrons varies from pixel to pixel, resulting in different gray levels. In practice, a single imaging electron can cause signals in more than one pixel because of multiple scattering within the scintillator material and the creation of an excitation volume. This effect is described by the point-spread function (PSF) of the detector, and its Fourier transform is the modulation-transfer function (MTF) [33–35].

The average number of electrons N_j collected by the jth detector pixel is

$$N_j = D\delta^2 I_j, \tag{4}$$

where D represents the electron dose, δ denotes the sampling (pixel size) and I_j is the probability of the electron hitting the jth pixel.

2. The actual number of electrons collected by each detector pixel is generated with random Poisson distribution, indicating that the standard deviation of the number of electrons collected by the jth detector pixel is $\sqrt{N_j}$.

The SNR of the whole image is evaluated as [36]

$$\overline{SNR} = \frac{\overline{N}}{\sigma(N)}, \tag{5}$$

where the average number of electrons per image pixel $\overline{N}$ is defined as

$$\overline{N} = \frac{1}{J}\sum_{j=1}^{J} N_j = \frac{D\delta^2}{J}\sum_{j=1}^{J} I_j = D\delta^2\overline{I}. \tag{6}$$

Here J is the total number of pixels and $\overline{I}$ is the average image intensity. $\sigma(N)$ is the standard deviation of the number of electrons collected by each pixel. We define the actual number of electrons collected by the jth image pixel as $Pois(D\delta^2 I_j)$, then

$$\sigma(N) = \sqrt{\frac{1}{J}\sum_{j=1}^{J}[Pois(D\delta^2 I_j) - \overline{Pois(D\delta^2 I_j)}]^2}. \tag{7}$$

If $I_j = \overline{I}$ for any image pixel, indicating the probability of the electrons hitting each image pixel is the same, then $\sigma(N) = \sqrt{D\overline{I}}\delta = \sqrt{\overline{N}}$ and $\overline{SNR} = \sqrt{\overline{N}}$.

2.2. Experimental setup for TEM imaging

Our modeling is based on the characteristics of the prototype SALVE II microscope. This system is based on a Zeiss Libra 200 MC equipped with a Schottky field emitter, an electrostatic Ω-type monochromator and an Ω-type in-column energy-filter. The TEM-platform has been optimized to achieve the highest objective lens current stability ($\Delta I/I < 10^{-7}$) within the voltage range between 20 and 80 kV [8]. The monochromator was used with the largest slit of 60 μm (basically no effect of monochromation) as C_c correction was applied. The size of the energy window of the filter was not limited by an energy-selecting slit but only by the physical limitations such as fixed apertures and tube diameters (about 130 eV at 40 kV). The SALVE II prototype is equipped with an aberration corrector to achieve atomic resolution even at low voltages of 20 and 40 kV, based on the design proposed by Rose [37]. Geometric axial aberrations are corrected up to the 5th order except for C_5, which was designed to be around 4 mm to obtain an optimized phase contrast transfer function. Off-axial aberrations are corrected up to the 3rd order for larger fields of view. The CMOS (complementary metal oxide semiconductor) based camera is the type TVIPS T416 (4k detector, $16 \times 16\ \mu m^2$ pixel size). The fiber-optics coupled scintillator was optimized to obtain large conversion rates for high sensitivity and very small thickness for high resolution.

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