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From 2D exit wave to 3D atomic structure

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The ultimate goal of electron microscopy is not to obtain nice images but to advance materials science. This means that EM has to evolve from describing to understanding materials properties. Understanding means matching observations with ab-initio calculations. And since all the structure-property relations are encoded in the positions of the atoms, they form the ultimate language between theory and experiment. The future EM is then to be considered as a communication channel between object and observer and the images as data planes from which the 3D atom positions can be extracted quantitatively. With the newest generation of Cs corrected EM's the resolution is sufficient to resolve the individual atoms and to refine their position with picometer precision. If the ideal object would be a phase object and the perfect electron microscope would have no aberrations, the HREM image intensity would show no contrast at all. Hence electron microscopic aberrations such as defocus are necessary to create contrast in the images. But on the other hand they scramble the information about the object. The best way to extract this information is by first undoing (deconvolving) the transfer functions of the electron microscope and the recording device. The first step is thus to retrieve the phase of the image wave. This can be done by off-axis electron holography or by focal series reconstruction, which is a kind of in-line holography. The next step is data mining the exit wave so as to retrieve the 3D positions of the object atoms. Since the exit wave is the result of the interaction of the electron wave with the object we need a physical model for this interaction that can be used for fitting. In general a 2D projection does not have sufficient information to retrieve 3D information so that one needs tomographic methods.

We can now consider two different cases: very thin objects and thicker crystalline objects.
In a very thin object we can consider the atom as point object which is the source of a spherical wave (Figure 1). By propagating over a certain distance *d*, the phases of the Fourier components of this wave increase linearly with distance and with the square of the spatial frequency *g*. Thus, by plotting the phase of the Fourier components versus g^2 we obtain a straight line. And from the slope we can then determine the distance *d* between the atom and the plane of observation. This is shown schematically in Figure 1. By analogy with the Hubble plot of cosmology we call this method big bang tomography. The experimental results of bilayer of grapheme are shown in Figure 2.

In case of a crystalline object viewed along a zone axis, the electrons are trapped in the positive potential of the atoms of the column and the propagation (channeling) of electrons is not influenced by the propagation in neighboring columns up to thicknesses of tens on nm, which are typical for HREM. This applies as well for perfect crystalline objects as for defective crystals with a column structure. Thus the exit wave of a crystalline object in a zone axis orientation represents the assembly of the exit waves of the constituting columns. Furthermore the atoms of a column act as weak lenses, which focus the electron wave periodically with depth so that the exit wave of a column is a very sensitive peaked fingerprint of the type of column. The theory of channelling is simple [2] and provides a way to interpret the exit wave, which can be visualized by plotting the complex values of the pixels in complex 2D space. From the exit wave of a column we can deduce the position of the column, the defocus distance (with sub-Angstrom precision), the total mass of the column and the residual aberrations [3].

By combining this information we can then reconstruct the object in 3D including profile of top and bottom surface. Figure 3 shows the Argand plot for a Ge crystal foil in (110) zone orientation. From the Argand plot we can determine the distance of the column to the exit wave and hence also the surface profiles.

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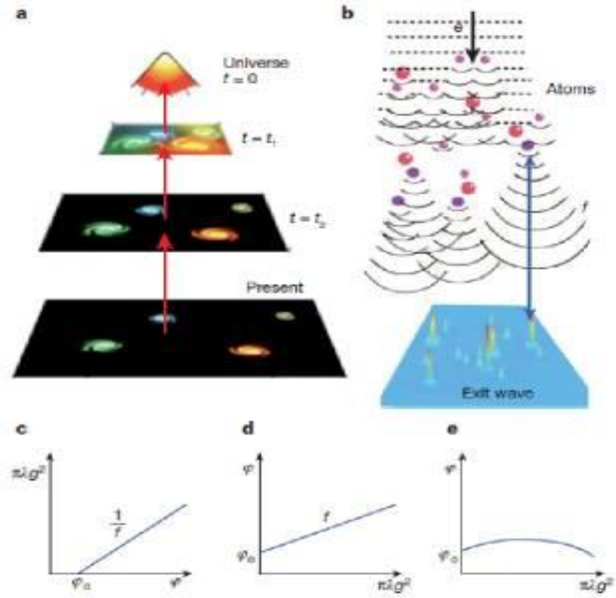

Figure 1. Big Bang analogy. a, b, Comparison between the Big Bang (a) and the point-atom 'big bang' (b). c, Phase speed plotted against phase. The relationship between the two is the same as that expressed in cosmology by Hubble's law, which gives the linear relationship between the distance and the speed of a distant galaxy. Here the slope is the reciprocal focal distance, 1/*f*. Note that at the position of the atom, the phase of the atom wave does not start from zero; instead, it has a value, φ_0, characteristic of the atom. d, Phase plotted against phase speed, which we refer to as the Hubble plot here. The slope gives the focal distance between the emitting atom and the plane of reconstruction of the exit wave. e, Same as in d, but with a minor residual spherical aberration with C_s = 50.3 µm (see text).

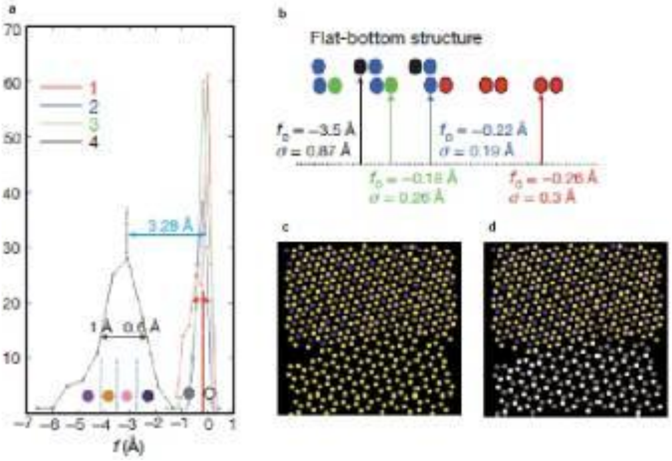

Figure 2. Histogram of the focal distance. **a**, Histogram of *f* for four different types of atom. **b**, the flat-bottom model. f_0, average focal distance, σ, standard deviation. **c**, Subtypes of atoms of type 4. **d**, Subtypes of atoms of type 1.

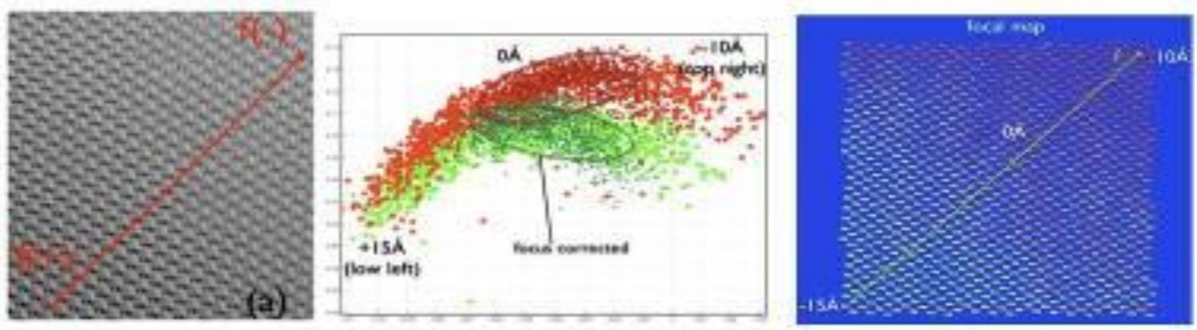

Figure 3. Experimental results for a Ge foil viewed along the (110) zone. Scale bar: 1 nm. From left to right: 1) amplitude of exit wave showing the peaks of the columns. 2) Argand plot showing two branches corresponding with the left (red) and the right (green) columns of the dumbbells. The separation between the two branches corresponds to a mass difference of 1 atom. 3) Defocus corrected phase image.