Quantitative analysis of wedge crystal structure based on the channelling theory

A. Wang[1], S. Van Aert[1], F. R. Chen[2], and D. Van Dyck[1]
1. EMAT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium
2. Department of Engineering and System Science, National Tsing Hua University, No. 101, Sec. 2, Kuang-Fu Road, 300 Hsinchu, Taiwan

amy.wang@ua.ac.be
Keywords: channelling theory, Argand plot, wedge structure, image simulation

In this abstract it will be shown that exit waves are very useful in order to obtain quantitative information on the projected atom column positions and on the composition of these columns. According to the channelling theory [1], the atom column acts as a channel for the incoming electrons in which the electrons scatter dynamically without leaving the column. The exit wave can be expressed analytically in a simple mathematical formula including only the lowest bound state, the 1s state, of the projected column potential [2]. A convenient way to visualize channelling theory is by plotting the complex value of the exit wave for each pixel located at a projected atom column position in a so-called Argand plot with the x- and y-coordinate corresponding to the real and imaginary value, respectively [3]. For a wedge-shape structure containing different thicknesses, the Argand plot is expected to yield a circular locus which starts at the origin (for zero thickness) and which has its center on the *x*-axis. The radius of the circle is then the amplitude of the scattering wave. As follows from the channelling theory, this radius should be identical for different atom column types if the columns are well-separated. The constant increments correspond to extra atoms in the column, and are different for different atom column types. For lighter atoms, the increment is smaller. From the plot, one can obtain the number of atoms in the column by counting the 'blobs'. More details about visualizing the structure information in exit wave from the Argand plot can be found in [4].

Ideally, the exit wave is the wave at the plane where the electron wave just leaves the atom columns. However, there is no such flat plane due to surface roughness (addition or deficiency of atoms comparing with neighboring columns). Practically, the exit wave can only be reconstructed in a plane which is close to the exit plane. However, there remains a gap between this plane and each atom column, which is different for every column. In other words, the defocus value for each atom column is different. In order to determine the defocus of each column, the exit wave of a particular column is defocused in the computer. This leads to an extra circular curve in the Argand plot, which we call the "defocus circle", as shown in Fig. 1(a). This curve may provide a simple method to determine the defocus of each column. In Fig. 1(b) it is shown that the defocus circles for atom columns containing different number of atoms pass through a common point. This reference wave point is common for all columns and corresponds to the entrance wave, ideally (1,0). Once the common point is known, a straight line from this point through the center of the defocus circle will intercept at zero defocus. The distance between the point of the column exit wave to this zero defocus point determines the defocus value of the atom column. Fig. 2(a) shows the defocus map for a top-flat wedge-shape structure with columns including 1 to 5 Au atoms. The simulated exit wave is taken at the plane where the electron wave leaves all atom columns, which is at the exit plane of the columns with 5 atoms. It is also clearly shown in Fig. 2(b) that the defocus

G. Kothleitner, M. Leisch (Eds.): MC2009, Vol. 1: Instrumentation and Methodology,
DOI: 10.3217/978-3-85125-062-6-015, © Verlag der TU Graz 2009

circles cross a common point. Note that this common point may be shifted in the presence of a background intensity caused by inelastic diffuse scattering.

The above theories and predictions are recently carried out on an experimental case: a Au[110] bridge structure. The exit wave is reconstructed from a focal-series of high resolution images taken at the TEAM (*Transmission Electron Aberration-corrected Microscope*). Fig. 3(a) shows the amplitude and phase of the reconstructed exit wave and (b) shows the Argand plot of all the columns. The blobs corresponding to the number of atoms in the columns are not yet clearly seen. This is partly due to the defocusing effect described before. However, correcting for this effect is not yet possible due to the presence of a varying background. Further analyses are in process to subtract this background correctly.

1. D. Van Dyck et al., Optik **93**(3) (1993) p103.
2. P. Geuens and D. Van Dyck, Ultramicroscopy **93** (2002) p179.
3. W. Sinkler and L.D. Marks, Ultramicroscopy **75** (1999), p251.
4. A. Wang et al., Proceedings of EMC 2008 vol. **1** (2008), p167.
5. The authors would like to thank Dr. C. Kisielowski for providing the experimental data from Berkeley. A. Wang and S. Van Aert are grateful to the Fund for Scientific Research – Flanders.

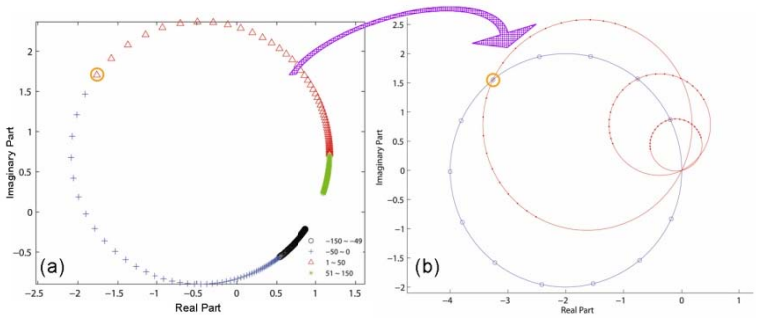

Figure 1. (a) Simulation of the defocus effect (from -150 Å to 150Å), which gives an extra defocus circle (b) for each thickness on the Argand plot.

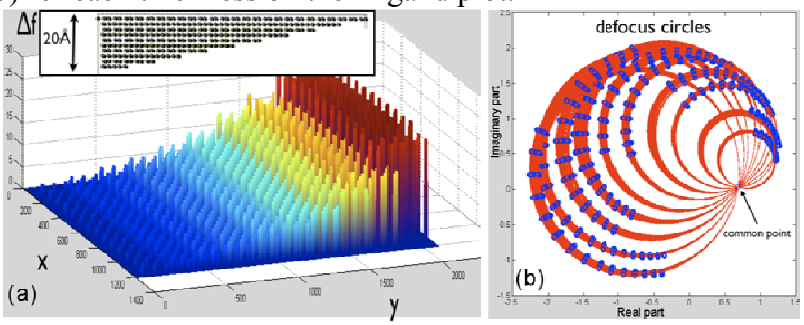

Figure 2. (a) The defocus map (Δf in Å) for a simulated top-flat wedge-shape structure (side view shown in the insert). (b) The defocus circles for each column. The circles pass through a common point.

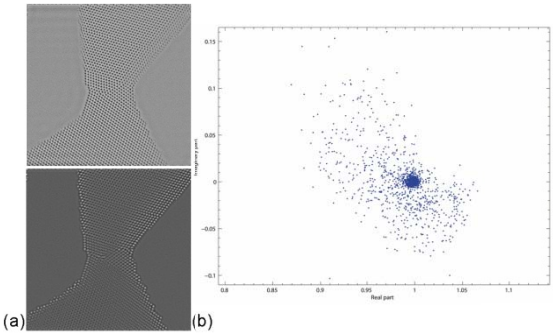

Figure 3. (a) Amplitude (top) and phase of the experiment Au[110] exit wave. (b) The Argand plot for each column.

DOI: 10.3217/978-3-85125-062-6-015,