CBED of strained materials

A. Chuvilin and U. Kaiser

Technical University Ilmenau, Centre for Micro-and Nanotechnology, Kirchhofstraße 7, 98693 Ilmenau, Germany

andrey.chuvilin@tu-ilmenau.de
Keywords: CBED, strain, simulation

Local strain field control is essential nowadays in many application fields including microelectronics devices and advanced internally stressed materials. During the last decade, with the development of subnano-sized electron probes, CBED was intensively exploited for this purpose [1-6]. The main intention to apply CBED for local strain analysis is that the area under analysis is thought to be of the size of the illuminating beam. This idea is based on the column approximation, which has been already discussed in the application to CBED [7].

We use a simple geometrical approach similar to [7] and dynamical simulation to demonstrate that the column approximation is not valid. The area of scattering of CBED pattern can exceed two orders of magnitude the size of the illuminating beam (Figure 1). Moreover, different HOLZ lines scatter from distinctly different areas of the sample (Figure 2) so that their positions at the central CBED disk correspond to lattice parameters from different parts of the crystal. Though such a scattering has no effect in the case of CBED from unstrained or uniformly strained crystal, it results in a number of serious consequences in the presence of a strain gradient. Among them are the line splitting and the symmetry violation (Figure 3), which are well known [4, 8, 9] and can be found in the most of the experimental papers on strain measurement by CBED. We demonstrate by dynamical simulations the influence of different strain distributions on the appearance and the arrangement of HOLZ lines at the central CBED disk.

It will be shown that strain measurement procedures based on fitting of HOLZ line positions in the presence of a strain gradient leads to incorrect results already at the gradient value as low as 10^{-5} nm^{-1}. Additional terms should be included in the expression for the HOLZ line shifts, accounting for the first and probably for the second derivatives of the strain field. This task does not seem to have a simple solution. The other approach could be to fit experimental data to dynamically simulated CBED for the model with strain distribution. However the drastically increased number of simulated parameters makes such fitting unreliable and unreasonably time consuming on the existing hardware.

We discuss further the possible computational and experimental workarounds for the problem, which may result in a completely new approach to strain field measurements by CBED.

1. H. Lakner, B. Bollig, S. Ungerechts, E. Kubalek, J. Phys. D: Appl. Phys. **29** (1996) p. 1767.
2. Y.Wakayama, Y.Takahashi, S.Tanaka, Jpn. J. Appl. Phys. **35** (1996) p. 1662.
3. R.Voelkl, U.Glatzel, M.Feller-Kniepmeier, Acta Mater **46** (1998) p. 4395.
4. S. Kraemer, J. Mayer, C. Witt, A. Weickenmeier, M. Ruhle, Ultramicroscopy **81** (2000) p. 245.
5. I. Berbezier, A. Ronda, A. Portavoce, J. Phys.: Condens. Matter **14** (2002) p. 8283.
6. I. De Wolf, V. Senez, R. Balboni, A. Armigliato, S. Frabboni, A. Cedola, S. Lagomarsino, Microelectronic Engineering **70** (2003) p. 425.
7. J. M Zuo, J. C. H. Spence,.Phil. Mag. A 68 (1993) p 1055.
8. F.Banhart, Ultramicroscopy **56** (1994) p.233.
9. R.Pantel, L. Clément, J. L. Rouvière, L.F.Tz. Kwakman, Microsc Microanal 9(Suppl 2) (2003) p.866.
10. The work has been supported by the German Research Foundation DFG.

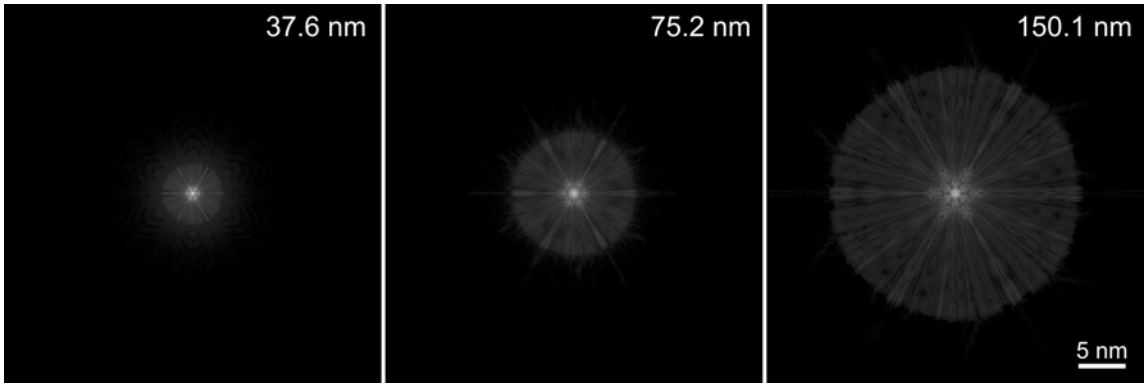

Figure 1 Amplitude of the electron wave propagating with the thickness (indicated at the up right corner) through Si in [111] direction, multislice simulation (100kV, initial beam size 0.3 nm, convergence semi angle 11 mrad, supercell 40x40 nm^2, matrix size 4Kx4K).

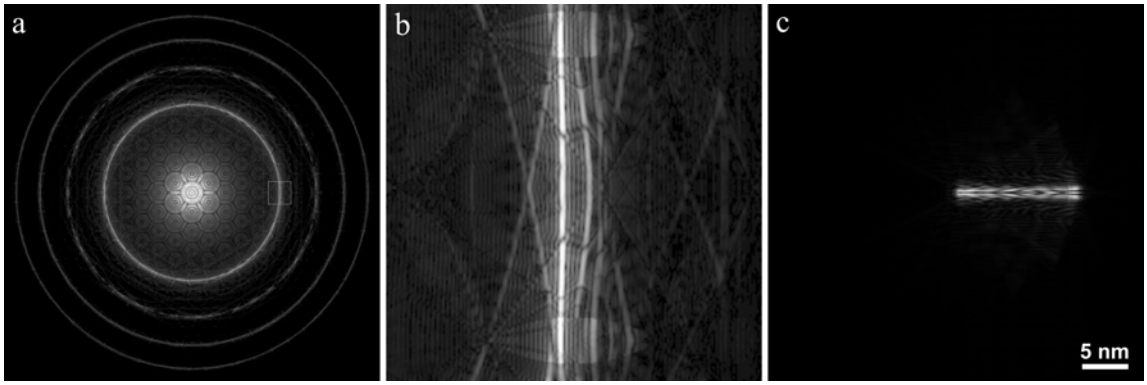

Figure 2 a) calculated CBED pattern corresponding to 150.1 nm thickness at Figure 1, b) enlargement of {5 5 –11} FOLZ line region (marked at (a)) demonstrating the well pronounced dispersion surface, c) dark field image reconstructed from the line (b) showing the area of line scattering (compare to Figure1 150.1 nm).

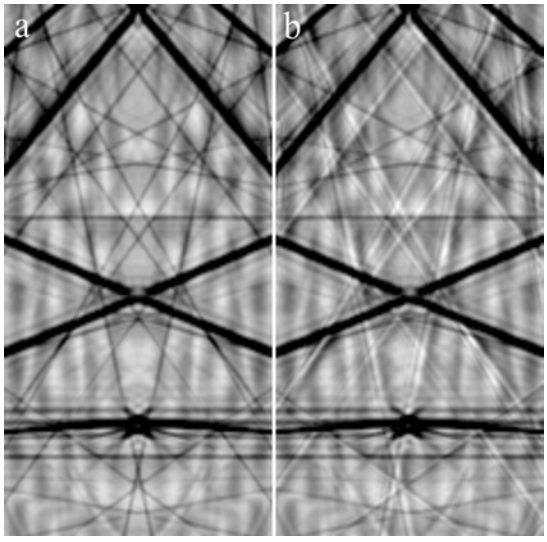

Figure 3 Areas of central disks of simulated CBED patterns for the [331] zone of Si at 100kV and 237 nm thickness: a) unstrained crystal, b) crystal strained in [110] direction with the gradient $5*10^{-4}nm^{-1}$ so, that the strain at the beam position is zero. The strain in [110] direction itself does not violate mirror plane, however the symmetry violation in CBED pattern cased by the strain gradient is clearly seen.