Oral Contributions

[MS22] Materials studied by (coherent) diffraction imaging

Co-Chairs: Ullrich Pietsch (DE), Simon Jacques (FR)

[MS22-03] Direct 3-dimensional atomic imaging by means of electron diffraction patterns

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Direct 3-dimensional imaging of atom arrangements is one of the most-wanted goals since Gabor has laid the foundation for holography in the late 1940s [1]. The necessary short wavelength for atomic resolution can be realised by using either radiation in the hard x-ray regime or by using electrons with kinetic energies above 150 eV. Compared to x-rays, electrons provide a very high scattering probability at neighboring atoms. Therefore, electron holography is very promising technique for studying organic molecules and, in its extended application for protein crystal structure search, since these systems mainly consist of light elements. We analyzed electron diffraction patterns of sample-internal electron sources in a holographic reconstruction scheme, since such pattern provide a rather high resolution as suggested by Szöke [2]. These internal-source diffraction patterns can be obtained from of x-ray photoelectron diffraction (XPD) [3,4]. XPD-patterns should yield a spatial image of the investigated structure on a atomic length scale, if an appropriate reconstruction scheme could be found. However, anisotropic electron scattering and multiple scattering effects [5,6] generally cause strong artifacts in the reconstruction. This, combined with twin image formation [7] prevented the reconstruction being interpreted as a clear image of the emitter environment. Here we present how to circumvent these problems by using electron diffraction patterns at electron kinetic energies of $E_{kin} \geq 10$ keV for the first time. Reconstructable electron diffraction patterns can also be obtained in the electron backscattering diffraction mode (EBSD [8]), since XPD-and EBSD-patterns are nearly identical in this energy range. We demonstrate that either XPD-or EBSD-patterns can be considered as holograms containing suffcient information for a successful reconstruction. Applying an adapted Fresnel-Kirchhoff integral, the reconstruction of these diffraction patterns results in a three-dimensional image function, with maxima perfectly matching to real atom locations. Here, the reconstruction scheme is a direct method for revealing the crystal structure without any further information needed. It is possible to identify atomic locations within a nanometer range in the reconstructed image since background noise and artifacts are rather weak. We present the images of up to a thousand atoms at their correct location for several different crystal systems. Starting on bcc-crystals we discuss the properties of the reconstruction scheme, turning to more complex systems as graphite with different emitter types, and polyatomic crystals. In all cases studied up to now, the spatial image reflected the respective crystal structure with all atoms at their correct location.

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