QUANTITATIVE ANALYSIS OF HIGH-RESOLUTION ELECTRON WAVE FUNCTIONS OF 2D MATERIALS

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Abstract

Usually the phase of the electron wave function is lost upon imaging in conventional transmission electron microscopy. In contrast to that the full electron wave function can be recorded by electron holography. Knowledge of amplitude and phase enables an a-posteriori elimination of residual aberrations and offers an increased information depth about a material's atomic structure.

Here, we present electron wave functions reconstructed from high-resolution off-axis electron holograms of two-dimensional samples of few-layer-thick WSe_2. We show that both microscope and sample-related parameters, such as image spread, specimen tilt and aberrations, can be obtained from comparisons between experimental wave functions and sophisticated simulations. The simulations are based on scattering potentials derived from density functional theory including bonding effects, which are found to be necessary to achieve a quantitative agreement between experimental and simulated amplitude and phase images [1].

The above-mentioned parameters are determined by comparing experimental and simulated wave functions on the same absolute scale. A precise knowledge of these parameters further enables us to draw conclusions about the object structure on the atomic scale. Hence, local structural defects can be detected even for specimen thicknesses of a few layers.

[1] S. Borghardt et al., Quantitative agreement between electron-optical phase images of WSe_2 and simulations based on electrostatic potentials that include bonding effects, submitted (2016)