HAADF STEM is used to determine structure parameters of nanostructures, such as the number of atoms and the atomic column positions. In order to quantitatively evaluate HAADF STEM images different performance measures including peak intensities and scattering cross sections have been introduced [1-3]. Here, a channelling based approach is proposed to predict these measures for mixed columns.

In the analysis of experimental images performance measures which are sensitive for the parameter of interest are desirable. A comparison between scattering cross sections, determined using statistical parameter estimation theory [2], and peak intensities shows that peak intensities level off at a relatively low number of atoms whereas scattering cross sections increase nearly linearly up to relatively large thicknesses (Fig. 1). This is in agreement with the scattering cross sections computed by using the probe-position integrated cross sections [3]. For that reason, the number of atoms of monotype atomic columns has been successfully determined from experimental scattering cross sections [4]. However, in case of mixed columns the analysis is more complicated since more structure parameters are involved. Therefore, it is desirable to be able to predict performance measures as a function of composition and thickness. Often the assumption of longitudinal incoherence is considered where the scattering intensity of an atomic column is written as the sum of the scattering intensities of the individual atoms constituting this column. However, the non-linear behaviour of peak intensities as well as scattering cross sections makes it impossible to make a valid prediction using this assumption (Fig. 2). A more accurate prediction is obtained based on the channelling theory in which it is assumed that each atom acts as a lens focussing the electrons on the next atom [5]. In this approach the change in scattering intensity with thickness of monotype atomic columns is taken with respect to that of a single atom to estimate the scattering intensity of mixed columns. This approach leads to a significant improvement in the prediction of both performance measures (Fig. 2) and is especially accurate for scattering cross sections. This is an important step forward for the quantitative analysis of complex hetero-nanostructures.

In conclusion, scattering cross sections of mixed columns can be predicted more accurately using a channelling based approach as compared to assuming longitudinal incoherent modelling.

References

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Fig. 1: Simulations of the scattering cross sections and peak intensities of a single atomic column of (a) Al, (b) Ag, (c) Cd and (d) Pb with respect to thickness. Simulations were carried out using an aberration corrected system with a convergence angle of 21.78 mrad and a detector covering an area of 90-158 mrad.

Fig. 2: Prediction models of simulated scattering cross sections and peak intensities for 17 atom thick mixed columns. In (a) and (c) the centre of an Al column is replaced by Ag atoms keeping the thickness at 17 atoms. In (b) and (d) the centre of a Cd column is replaced by Pb atoms. The parameters for the simulations were the same as in Fig. 1.