ABSORPTION EDGE MODELING IN LINE PROFILE FITTING APPLICATIONS

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Kß-filters are the most frequently used devices for monochromatization of X-rays in laboratory diffractometers. Monochromatization is based on the K absorption edge of the employed filter material to selectively allow transmission of the Kα characteristic lines while filtering Bremsstrahlung, Kß radiation and other characteristic lines. The major disadvantage of Kß filters is that they introduce absorption edges at the low energy side of diffraction peaks, dependent on the wavelength/filter material and its thickness. With position sensitive detectors (PSDs) absorption edges are much more pronounced due to the high intensity data typically collected; while for point detectors absorption edges usually are obscured by counting statistics, absorption edges are clearly visible in most patterns recorded using PSDs. In traditional profile fitting procedures absorption edges frequently prevent the accurate description specifically of peaks tail regions, und thus often represent a major part of the remaining misfit to the data, specifically at low angles 2θ.

In this paper we will introduce a new approach to accurately model absorption edges as implemented in line profile fitting applications. This is achieved by

1. Extending source emission profiles to include transmitted Kß and Bremsstrahlung, adaptively damped by the transmission of the filter material
2. Blending of the resulting peak profile function with a filter function considering

a) the position of the absorption edge according to the respective filter material,
b) the change of transmission at the respective energy of the absorption edge,
c) the amplitude of the filter function according to the transmission (thickness) of the respective filter material
d) a broadening of the sharp transmission edge of the step function that is related to the real micro-structure of the sample

This refinement model allows an excellent fit to absorption edges with significantly lowered R_{WP}. More reliable size-strain parameters will be obtained due to the improved modelling of peak tail regions. The same holds for quantitative phase analysis when peaks of minor phases are located close to absorption edges. Several examples will be discussed for Cu and Mo radiation.