Parametrizations for Scattering Potentials in high-energe TEM

It should be noted that every quantity is in SI-units, regardless of what the originators of the parametrizations used. Also the spatial frequency is in the proper unit $k = \frac{2\pi}{\lambda}$.

1 Weickenmeier-Kohl

This parametrization is from the paper: Weickenmeier and Kohl, "Computation of absorptive form factors for high-energy electron diffraction" in Acta Cristallographica 1991.

The atoms are paremtrized by 7 factors, which we will call A_0 and $B_1, ..., B_6$ and can be found in the corresponding parameters file "../parameters/weickenmeier_kohl_coefficients.dat".

$$A_1 = A_2 = A_3 = \frac{16\pi^2 \cdot 2.395e8 \cdot Z}{3(1 + A_0)} \tag{1}$$

$$A_4 = A_5 = A_6 = A_0 A_1 \tag{2}$$

$$F(\mathbf{k} \neq 0) = \sum_{i=1}^{6} A_i \frac{\left(1 - e^{-B_i \mathbf{k}^2}\right)}{k^2} \tag{3}$$

$$F(\mathbf{k} = 0) = \sum_{i=1}^{6} A_i B_i \tag{4}$$

2 Weickenmeier-Kohl as seen in FSCATT

3 Kirkland

This parametrization is from the book: Earl Kirkland, "Advanced Computing in Electromn Microscopy", 1998.

The atoms are paremtrized by 16 factors, which we will call $A_1, ..., A_4$, $B_1, ..., B_4$, $C_1, ..., C_4$ and $D_1, ..., D_4$ and can be found in the corresponding parameters file "../parameters/kirkland_coefficients.dat".

$$F(\mathbf{k}) = \sum_{i=1}^{4} \frac{A_i}{\frac{\mathbf{k}^2}{4\pi^2} + B_i} + \sum_{i=1}^{4} C_i e^{-D_i \frac{\mathbf{k}^2}{4\pi^2}} \tag{5}$$

$$\tag{6}$$

4 Peng-Dudarev