

Parametrizations for Scattering Potentials in high-energy 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 units, therefore $k = \frac{2\pi}{\lambda}$.

1 Weickenmeier-Kohl

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

The atoms are parametrized by 7 factors, which we will call A_0 and B_1, \dots, B_6 and can be found in the corresponding parameters file “../parameters/weickenmeier_kohl_coefficients.dat”.

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

$$A_4 = A_5 = A_6 = A_0 A_1 \quad (2)$$

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

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

2 Weickenmeier-Kohl as seen in FSCATT

3 Kirkland

This parametrization is from the book: Earl Kirkland, “Advanced Computing in Electron Microscopy”, 1998.

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

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

(6)

4 Peng-Dudarev

The atoms are parametrized by 10 factors, which we will call $A_0, \dots, A_4, B_0, \dots, B_4$ and can be found in the corresponding parameters file “../parameters/kirkland_coefficients.dat”. As the parameters have not been converted properly there is still the conversion factor $c = 1 \cdot 10^{-20}$ in the exponents.

$$F(\mathbf{k}) = \sum_{i=0 \dots 5} A_i \exp(-B_i c \mathbf{k}^2) \quad (7)$$

5 Wentzel, with Thomas-Fermi screening

The potentials are parametrized purely by the Z of the atoms.

$$V(\mathbf{r}) = -\frac{2\gamma Z}{a_0} \frac{e^{-|\mathbf{r}|/R}}{|\mathbf{r}|} \quad (8)$$