

Table 1: Name, definition, and  $d_{hkl}$  of the models available for simulation.

Name	Definition	Adjustable parameters	$d_{hkl}$
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	a, b, c $\alpha, \beta, \gamma$	$\frac{1}{\sqrt{\frac{h^2}{a^2} \sin^2 \alpha + \frac{k^2}{b^2} \sin^2 \beta + \frac{l^2}{c^2} \sin^2 \gamma - \frac{2kl}{bc} (\cos \alpha - \cos \beta \cdot \cos \gamma) - \frac{2lh}{ca} (\cos \beta - \cos \gamma \cdot \cos \alpha) - \frac{2hk}{ab} (\cos \gamma - \cos \alpha \cdot \cos \beta)}}$
Monoclinic	$a \neq b \neq c$ $\alpha = \beta = \pi/2$ $\gamma \neq \pi/2$	a, b, c $\gamma$	$\frac{\sin \gamma}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2 \sin^2 \gamma}{c^2} - \frac{2hkc \cos \gamma}{ab}}}$
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = \pi/2$	a, b, c	$\frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$
Hexagonal	$a = b \neq c$ $\alpha = \beta = \pi/2$ $\gamma = 2\pi/3$	a, c	$\frac{1}{\sqrt{\frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}}}$
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = \pi/2$	a, c	$\frac{a}{\sqrt{h^2 + k^2 + l^2 \frac{a^2}{c^2}}}$
Cubic	$a = b = c$ $\alpha = \beta = \gamma = \pi/2$	a	$\frac{a}{\sqrt{h^2 + k^2 + l^2}}$

Table 2: Extinction rules available for different lattice types

Lattice type	Extinction rule	Availability
Primitive	None	All
Body centered	$h + k + l = 2n + 1$ (odd)	Cubic, Tetragonal, Orthorhombic
Face centered	h, k and l have different parities	Cubic, Orthorhombic
Base centered (c)	$h + k = 2n + 1$	Orthorhombic
Hexagonal (HCP)	$l = 2n + 1$ (odd) AND $h + 2k = 3n$	Hexagonal