Cheat Sheet for Diffraction Experiments

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2θ is the scatering angle, but not always a diffractometer axis. θ is (sometimes) a diffractometer axis. Their difference is called omega:

$$\omega = \theta - (2\theta)/2 \tag{1}$$

Bragg's Law

$$\lambda = 2d\sin(2\theta/2) \tag{2}$$

Scattering Vector/Momentum Transfer

$$Q = 2\pi/d = \frac{4\pi\sin(2\theta/2)}{\lambda} \tag{3}$$

Miller indices

$$h = \frac{q_x a}{2\pi} \tag{4}$$

$$k = \frac{q_y b}{2\pi} \tag{5}$$

$$\ell = \frac{q_z c}{2\pi} \tag{6}$$

Length scale c_{actual} of diffraction feature at ℓ_{actual} compared to reference length scale c_{ref} at ℓ_{ref} (which, e.g., comes from orientation matrix):

$$c_{actual} = c_{ref}\frac{\ell_{ref}}{\ell_{actual}} \tag{7}$$

Debye-Waller factor

$$e^{-M} = e^{-Bq^2/(16\pi^2)} = e^{-<u^2>q^2/2} \tag{8}$$

Constants

$$hc/e = 12.398424 \text{ Å keV} \tag{9}$$

Lattice Parameters

$$a_{diamond} = 3.56688 \text{ Å} \tag{10}$$

$$a_{Si} = 5.43102 \text{ Å} \tag{11}$$

$$a_{Ge} = 5.65795 \text{ Å} \tag{12}$$

$$a_{GaAs} = 5.65325 \text{ Å} \tag{13}$$

$$a_{MgO} = 4.2198 \text{ Å} \tag{14}$$