G

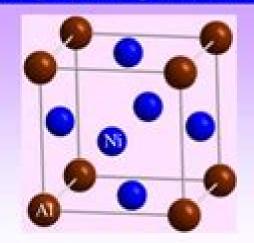
SC, Al at (0,0,0), Ni at (1/2, 1/2, 0) and equivalent positions

(1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2)

$$F = f_{Al} \left[e^{i[2\pi(0)]} \right] + f_{Nl} \left[e^{i[2\pi(\frac{h+k}{2})]} + e^{i[2\pi(\frac{k+l}{2})]} + e^{i[2\pi(\frac{l+h}{2})]} \right]$$

$$= f_{Al} + f_{Nl} \left[e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)} \right]^{\frac{1}{2} - \frac{1}{2}}$$
Real

Simple Cubic (L12 ordered structure)



$$F = f_{Al} + f_{Nl} [e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)}]$$

(h, k, l) unmixed

h,k,l → all even or all odd

(h, k, l) mixed

 $F = f_{Al} + 3f_{Nl} + F^2 = (f_{Al} + 3f_{Nl})^2 (111), (200), (220), (333), (420)$

$$F = f_{AI} - f_{NI} \rightarrow F^2 = (f_{AI} - f_{NI})^2$$
 (100), (211); (210), (032), (033)

Two odd and one even (e.g. 112); two even and one odd (e.g. 122)

Numerical Structure Factor Tables

Camilla Rothe

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