

1.45: Flack parameter

The Flack parameter is the molar fraction x in the defining equation $C = (1 - x)X + x\bar{X}$, where C represents an oriented two-domain-structure crystal, twinned by inversion, consisting of an oriented domain structure X and an oriented inverted domain structure \bar{X} . In reciprocal space, the Flack parameter x is defined by the structure-amplitude equation

$$G^2(h, k, l, x) = (1 - x)|F(h, k, l)|^2 + x|F(\bar{h}, \bar{k}, \bar{l})|^2.$$

For a multidomain-structure twin of a chiral crystal structure, an equivalent Flack parameter may be calculated according to the method of Flack and Bernardinelli (1999).

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