

The relation of anisotropic peak broadening with lattice symmetry in powder diffraction

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Lattice relaxation, i.e. small lattice symmetry lowering, could lead to unresolved peak splitting in powder diffraction, which results in anisotropic, i.e. hkl -dependent, peak broadening. Recently Gregorkiewicz & Boschetti [1] derived formulas for $1/d_{hkl}^2$ (with d_{hkl} being an interplanar distance) for each split peak component in the following minimal relaxation schemes: (i) cubic to tetragonal, (ii) cubic to rhombohedral, (iii) hexagonal to orthorhombic/monoclinic, (iv) tetragonal to orthorhombic, (v) orthorhombic to monoclinic, (vi) monoclinic to anorthic (triclinic). Anisotropic peak broadening caused by lattice relaxation can be parameterized by the variance of those slightly dispersed peaks' positions [2]. For all relaxation schemes the variances $\sigma^2(h, k, l)$ are expressed as fourth-order polynomials in h, k, l indices [2]:

$$\sigma^2(h, k, l) = \sum_{HKL} S_{HKL} h^H k^K l^L,$$

with $H + K + L = 4$. Popa [3] provided symmetry restrictions for each Laue class for S_{HKL} coefficients. Stephens' phenomenological model of anisotropic peak broadening [4] assumes that each crystallite in a powder sample is generally triclinic and that only the average lattice constants over the entire sample satisfy the restrictions of a given lattice symmetry. Consequently, peak broadening can also be expressed as fourth-order polynomials in h, k, l . However, anisotropic peak broadening caused by the lattice relaxation gives more constraints [2] between the S_{HKL} coefficients as compared with those listed in [3, 4]. The seminal papers by Popa [3] and Stephens [4] and the recent paper by Gregorkiewicz & Boschetti [1] are connected by expressing the S_{HKL} parameters in terms of lattice parameter increments [2].

[1] Gregorkiewicz, M. & Boschetti, A. (2024). *Acta Cryst. A* **80**, 439.

[2] Fabrykiewicz, P. (2025) *Acta Cryst. A* **81**, 245.

[3] Popa, N. C. (1998). *J. Appl. Cryst.* **31**, 176.

[4] Stephens, P. W. (1999). *J. Appl. Cryst.* **32**, 281.

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