For Laue symmetries other than triclinic, there are restrictions on the allowed S_{hkl} terms and, as a practical matter, additional equivalences from symmetry-forced reflection overlaps for trigonal and tetragonal Laue symmetries.

Monoclinic (2/m, b axis unique; others similar, nine coefficients):

$$\Gamma^2_{sL} = S_{400}h^4 + S_{040}k^4 + S_{004}l^4 + 3S_{202}h^2l^2 + 3(S_{220}h^2k^2 + S_{022}k^2l^2) + 2(S_{301}h^3l + S_{103}hl^3) + 4S_{121}hk^2l. \quad (3.3.34)$$

Orthorhombic (mmm, six coefficients):

$$\Gamma^2_{sL} = S_{400}h^4 + S_{040}k^4 + S_{004}l^4 + 3(S_{220}h^2k^2 + S_{202}h^2l^2 + S_{022}k^2l^2). \quad (3.3.35)$$

Tetragonal (4/m, five coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4) + S_{004}l^4 + 3S_{220}h^2k^2 + 3S_{202}(h^2l^2 + k^2l^2) + 2S_{310}(h^3k - hk^3). \quad (3.3.36)$$

The last coefficient (S_{310}) cannot normally be determined owing to exact reflection overlaps. Thus, equation (3.3.37) is normally used for both 4/m and 4/mmm Laue symmetries:

Tetragonal (4/mmm, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4) + S_{004}l^4 + 3S_{220}h^2k^2 + 3S_{202}(h^2l^2 + k^2l^2). \quad (3.3.37)$$

Trigonal ($\bar{3}$, rhombohedral setting, five coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + l^4) + 3S_{220}(h^2k^2 + h^2l^2 + k^2l^2) + 2S_{310}(h^3k + k^3l + hl^3) + 2S_{130}(h^3l + kl^3 + hl^3) + 4S_{211}(h^2kl + hk^2l + hkl^2). \quad (3.3.38)$$

The pair of coefficients S_{310} and S_{130} cannot normally be independently determined owing to exact reflection overlaps. Thus, equation (3.3.39) is normally used for both rhombohedral symmetries:

Trigonal ($\bar{3}m$, rhombohedral setting, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + l^4) + 3S_{220}(h^2k^2 + h^2l^2 + k^2l^2) + 2S_{310}(h^3k + k^3l + hl^3 + h^3l + kl^3 + hl^3) + 4S_{211}(h^2kl + hk^2l + hkl^2). \quad (3.3.39)$$

Trigonal ($\bar{3}$, five coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2) + S_{301}(2h^3l - 2k^3l - 6hk^2l) + 4S_{211}(h^2kl + hk^2l). \quad (3.3.40)$$

The coefficient S_{301} cannot normally be independently determined owing to exact reflection overlaps. Thus, equation (3.3.42) is normally used for $\bar{3}$ Laue symmetry.

Trigonal ($\bar{3}m1$, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2) + S_{301}(3h^2kl - 3hk^2l + 2h^3l - 2k^3l). \quad (3.3.41)$$

The coefficient S_{301} cannot normally be independently determined due to exact reflection overlaps. Thus, equation (3.3.43) is normally used for $\bar{3}m1$ Laue symmetry.

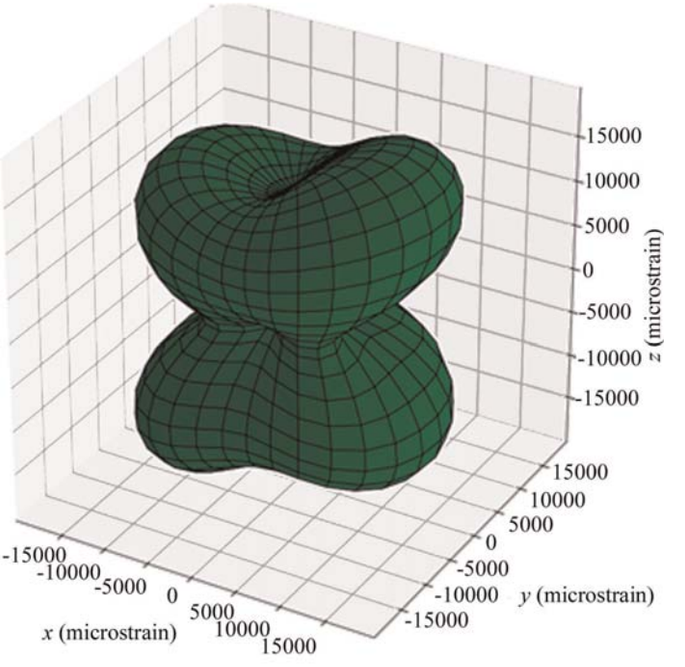

Figure 3.3.4
Microstrain surface for sodium parahydroxybenzoate multiplied by 10^6.

Trigonal ($\bar{3}1m$, four coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2) + 4S_{211}(h^2kl + hk^2l). \quad (3.3.42)$$

Hexagonal (6/m and 6/mmm, three coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + 2h^3k + 2hk^3 + 3h^2k^2) + S_{004}l^4 + 3S_{202}(h^2l^2 + k^2l^2 + hkl^2). \quad (3.3.43)$$

Cubic ($m\bar{3}$ and $m\bar{3}m$, two coefficients):

$$\Gamma^2_{sL} = S_{400}(h^4 + k^4 + l^4) + 3S_{220}(h^2k^2 + h^2l^2 + k^2l^2). \quad (3.3.44)$$

These equations can be used with the refined values of the coefficients to produce a surface representing the extent of the microstrain in reciprocal space. The surface resulting from Stephens' (1999) analysis of powder diffraction data from sodium parahydroxybenzoate is shown Fig. 3.3.4. At the present time, the connection between the elastic properties and defects with these microstrain surface models is unclear. Some aspects of this for cubic and hexagonal systems are discussed in Chapter 5.1.

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