Appendix (to be deposited online)

The following lines were used within a "str" phase (structure phase; conventional Rietveld refinement) within the "Launch mode" of TOPAS (Bruker AXS, 2006) to describe phenomenologically the microstrain broadening as described in section 2.1. The refined user-defined parameters z1111 etc. (lines 1-6) correspond to the parameter Z_{1111}^{B} etc. scaled by a factor of kk = 10^8 (line (11); i.e. the present Z parameters have to be multiplied by 10^{-8} to obtain the real, physical Z parameters). xx, yy and zz (lines 8-10) correspond to x_1, x_2 and x_3, i.e. the projection of the unit vector parallel to the diffraction vector in the Cartesian frame of reference with basis vectors parallel to **a**, **b**, and **c**. In terms of the parameters used in the present paper line (8) would e.g. read $x = d_{hkl} \cdot h/a$. The parameter ee in line (11) corresponds to the *hkl*-dependent squared Full-Width-at-Half-Maximum of the microstrain distribution along the diffraction vector, $B^2_{\Delta\varepsilon_{hkl}}$, compare Eq. (7) in the main paper. The parameter pp in line (12) is the squared FWHM of the line-broadening contribution (factor of 180/π in order to obtain the required value in degrees 2θ) due to microstrain for the reflection *hkl*, $B^2_{\Delta 2\theta_{hkl}}$ in Eq. (6). This FWHM refers to a pseudo Voigt function (mixing parameter η : etax; defined in line (13)) which is convoluted (line (14)) with the employed description of the instrumental resolution function.

prm z1111 15979.81122` min 0 (1)

prm z2222 250901.49094` min 0 (2)

prm z3333 12855.77740` min 0 (3)

prm z1122 8444.20964` (4)

prm z1133 43881.35349` (5)

prm z2233 521.39418` (6)

prm !kk = 10^(-8); (7)

prm xx = D_spacing H/Lpa; (8)

prm yy = D_spacing K/Lpa; (9)

prm zz = D_spacing L/Lpc; (10)

prm ee = kk (z1111 xx^4 +z2222 yy^4 + z3333 zz^4 + 6 z1122 xx^2 yy^2 + 6 z1133 xx^2 zz^2 + 6 z2233 yy^2 zz^2); (11)

prm pp = (-2 Tan(Th))^2 ee; (12)

prm etax 0.44089 min 0 max 1.2 (13)

user_defined_convolution =
(1-etax) (Ln(16)/3.1415927)^.5 1/pp^.5 Exp(-Ln(16) X^2/(pp))
+ 2 etax/3.1415927/pp^.5 1/(4 X^2/pp+1); min -2 max 2 (14)