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ARTICLE TYPE

Defect accommodation in nanostructured soft crystals (Supporting Information)

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Azimuthal peak shape function

If the peak shapes are mainly determined by the radial and azimuthal peak shapes, the peak shape function can be factorized into a radial part $L_q(q, g_{hkl})$ depending on the modulus of the scattering vector, and an azimuthal part $L_\psi(q, g_{hkl}, \psi_{hkl})$ depending on the angle $\psi_{hkl} = \arccos\left(g_{hkl}\,q/\left(|g_{hkl}||q|\right)\right)$ between the scattering vector and the reciprocal lattice vector such that

$$L_{hkl}(\mathbf{q}, \mathbf{g}_{hkl}) = L_q(q, g_{hkl})L_\psi(q, g_{hkl}, \psi_{hkl}) \qquad \text{(S1)}$$

The normalized radial peak shape functions are given by

$$L_q(q, g_{hkl}) = \begin{cases} \dfrac{2}{\pi\delta_q}\exp\left[-\dfrac{4(\mathbf{q}-\mathbf{g}_{hkl})^2}{\pi\delta_q^2}\right] & \text{Gaussian} \\ \dfrac{\delta_q}{2\pi}\left(1+\dfrac{4(\mathbf{q}-\mathbf{g}_{hkl})^2}{\delta_q^2}\right)^{-1} & \text{Lorentzian} \end{cases} \qquad \text{(S2)}$$

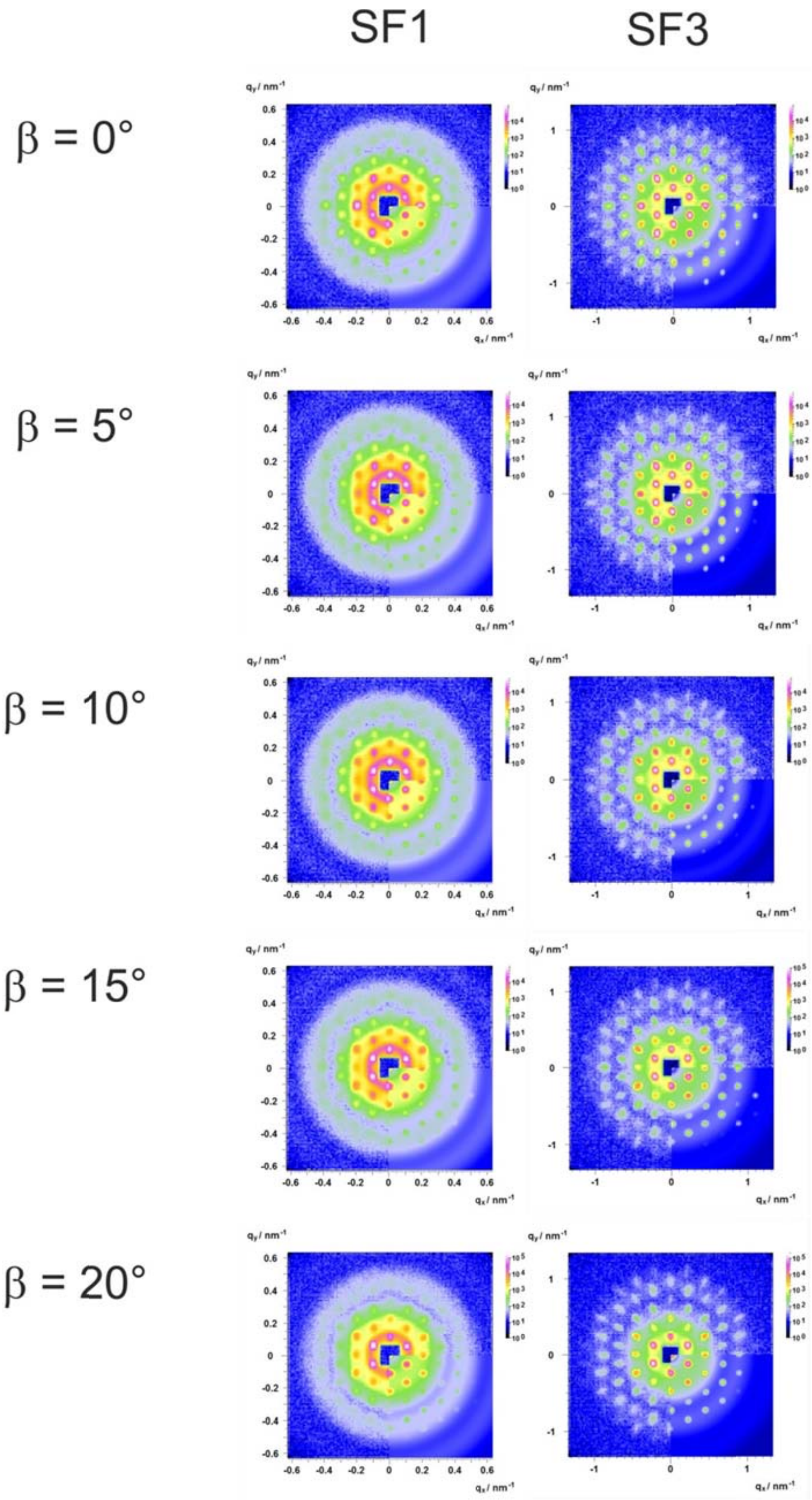
where δ_q is the radial peak width which in case of a Lorentzian is equal to the full width at half maximum (FWHM). For a Gaussian it is related to the standard deviation as $\sigma_q = \sqrt{\pi/8}\,\delta_q$. Other peak shapes such as Pseudo-Voigt or Pearson VII did not lead to significant improvements in the simulations outlined below.

The normalized azimuthal peak shape functions are given by

$$L_\psi(q, g_{hkl}, \psi_{hkl}) = \begin{cases} \dfrac{1}{2\pi g_{hkl}^2 K(a_{hkl})}\exp\left[-\dfrac{4\psi_{hkl}^2 q^2}{\pi\delta_\psi^2}\right] & \text{Gaussian} \\ \dfrac{1}{2\pi g_{hkl}^2 K(b_{hkl})}\left(1+\dfrac{4\psi_{hkl}^2 q^2}{\pi\delta_\psi^2}\right)^{-1} & \text{Lorentzian} \end{cases} \qquad \text{(S3)}$$

with $a_{hkl} = \dfrac{4g_{hkl}^2}{\pi\delta_\psi^2}$ and $b_{hkl} = \dfrac{4g_{hkl}^2}{\delta_\psi^2}$. $K(a_{hkl})$ and $K(b_{hkl})$ are normalization functions which are derived in Ref. [23] In the isotropic limit $(a_{hkl}, b_{hkl} \to 0)$ the azimuthal peak shape functions reduce to $L_\psi(g_{hkl}) = \left(4\pi g_{hkl}^2\right)^{-1}$.

Complete set of scattering patterns



Electronic Supplementary Material (ESI) for Nanoscale

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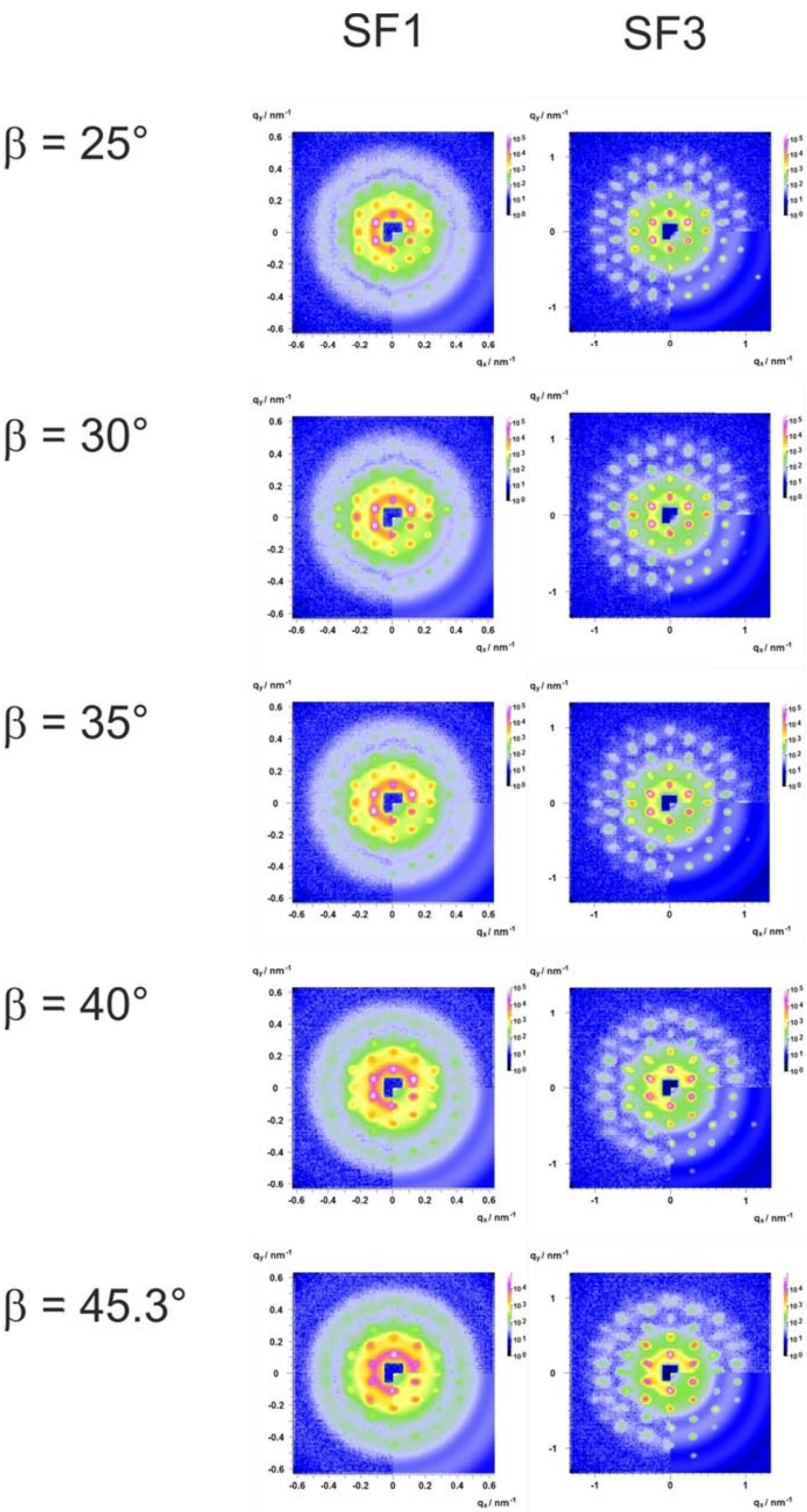

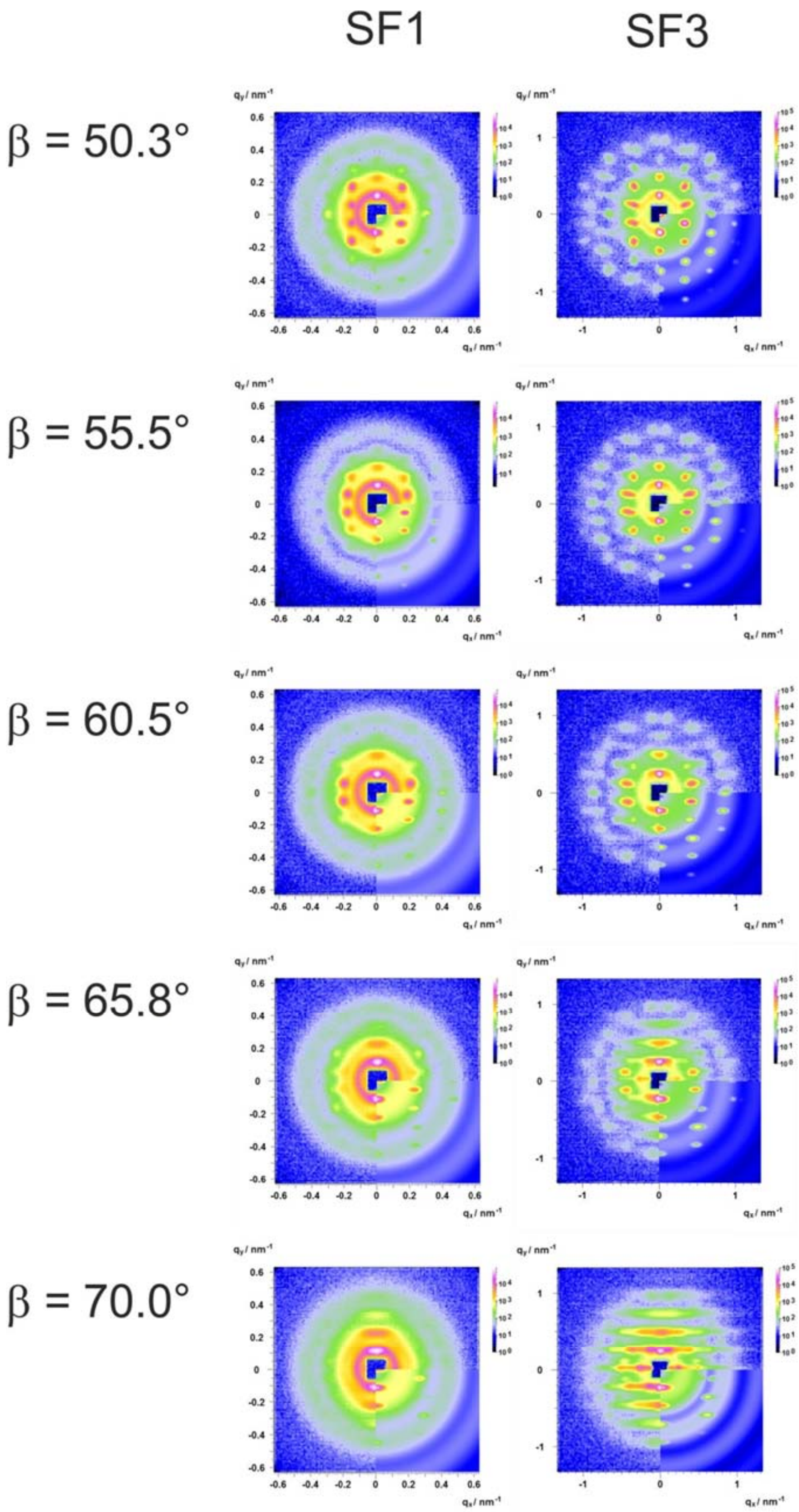
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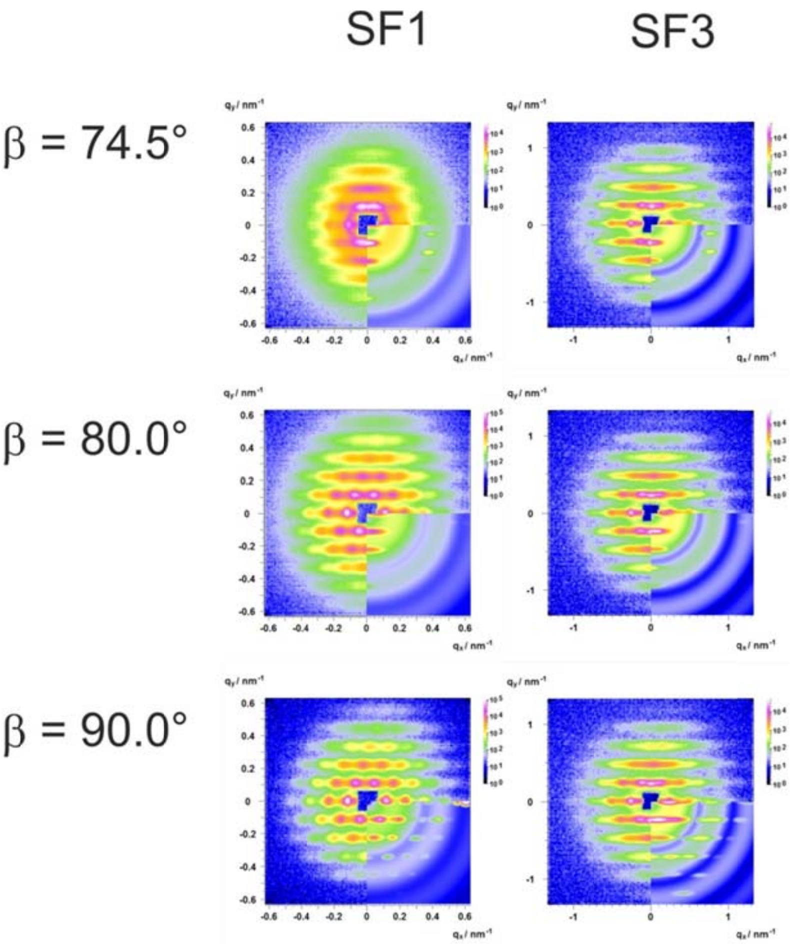
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