JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 55 (2022)

Supporting information for article:

Orientation evaluation of the UHMWPE fibers: previous studies and an improved method

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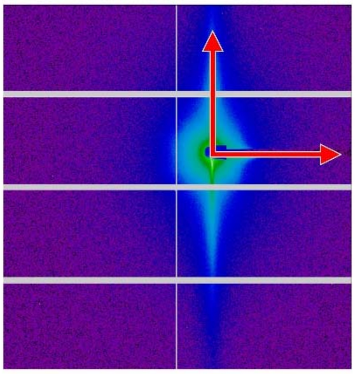

Fig.1 Definition of directions in USAXS pattern.

To illustrate the calculated method, the fiber axis, meridional and equatorial direction of SAXS patterns were defined in Fig.1

Considering that the length of the microfiber (L) is much larger than width (D), we can approximately consider it as a needle-like structure. The intensity distribution of microfibers with uniaxial preferred orientation is given by[1]

$$I(s,\phi) = n\rho_{\mathrm{m}}^2 \int_0^{\frac{\pi}{2}} I_{\mathrm{v}}(s,\phi')F(\phi,\phi')\sin\phi' d\phi' \quad (1)$$

$$F(\phi,\phi') \propto \int_0^{\pi} g_{\mathrm{ax}}(\beta)\mathrm{d}\eta \quad (2)$$

$$\cos\beta = \cos\phi\cos\phi' + \sin\phi\sin\phi'\cos\eta \quad (3)$$

where n is the number of microfibers. $F(\phi,\phi')$ is the orientation distribution ("pole figure") as a function of ϕ for the direction ϕ' in a system with simple fiber symmetry. $g_{\mathrm{ax}}(\beta)$ is the orientation distribution of the long axes of the microfibers. Accordingly, $g_{\mathrm{ax}}(\beta) \propto \mathrm{F}(\phi,0)$ and the corresponding equatorial distribution $g_{\mathrm{ep}}(\phi) \propto \mathrm{F}(\phi, \pi/2)$.

Because of L ≫ D and $g_{\mathrm{ep}}(\phi)$ is a relatively narrow distribution centered on $\phi = \pi/2$, we can use the approximations:

$$F\left(\phi,\frac{\pi}{2}-\Delta\phi'\right) \propto g_{\mathrm{eq}}(\phi-\Delta\phi') + g_{\mathrm{eq}}(\phi+\Delta\phi') \quad (4)$$

$$I_{\mathrm{v}}\left(s,\frac{\pi}{2}-\Delta\phi'\right) = \rho_{\mathrm{m}}^2|\Phi_D|^2(s\cos\Delta\phi')|\Phi_L|^2(s\sin\Delta\phi') \quad (5)$$

Furthermore, since $\Delta\phi'$ is considered to be small, we put cos $\Delta\phi' \approx 1$ and sin $\Delta\phi' \approx \Delta\phi'$, which results in:

$$I_{\mathrm{v}}\left(s,\frac{\pi}{2}-\Lambda\phi'\right) \simeq \rho_{\mathrm{m}}^{2}|\Phi_D|^2(s)|\Phi_L|^2(s\Delta\phi') \tag{6}$$

Considering the symmetry of $F(\phi,\pi/2-\Delta\phi')$ and $g_{\mathrm{ep}}(\phi)$, we can rewrite as:

$$I(\mathrm{s},\phi) = n\rho_{\mathrm{m}}^{2}|\Phi_D|^2(s)\int|\Phi_L|^2(s\Delta\phi')g_{\mathrm{eq}}(\phi-\Delta\phi')\mathrm{d}\Lambda\phi' \tag{7}$$

$$I(s,\phi) = n\rho_{\mathrm{m}}^{2}|\Phi_D|^2(s)\left[|\Phi_L|^2(s\phi)_{\phi}g_{\mathrm{eq}}(\phi)\right] \tag{8}$$

For the evaluation, we choose two functions, first the tangential width of the equatorial distribution $B_{\pi/2}(s)$ and, second, the scattering on the equator. Since the integral over g_{ep} is considered as constant, the latter expression can be simplified as:

$$\begin{aligned} B_{\frac{\pi}{2}}(s) &= \frac{1}{I\left(s,\frac{\pi}{2}\right)}\int I(s,\phi)\mathrm{d}\phi \\ &= \frac{\int\left[|\Phi_L|^2(s\phi)_{\phi}^{*}g_{\mathrm{eq}}(\phi)\right]\mathrm{d}\phi}{\left[|\Phi_L|^2(s\phi)_{\phi}g_{\mathrm{eq}}(\phi)\right]\left(\frac{\pi}{2}\right)} \end{aligned} \tag{9}$$

$$I\left(s,\frac{\pi}{2}\right) = n\rho_{\mathrm{m}}^{2}|\Phi_D|^2(s)\frac{1}{B_{\frac{\pi}{2}}(s)}\left[\int|\Phi_L|^2(s\phi)\mathrm{d}\phi\right]\times\left[\int g_{\mathrm{eq}}(\phi)\mathrm{d}\phi\right] \tag{10}$$

$$I\left(s,\frac{\pi}{2}\right) \propto n\rho_{\mathrm{m}}^{2}\frac{L}{sB_{\frac{\pi}{2}}(s)}|\Phi_D|^2(s) \tag{11}$$

$$\int|\Phi_L|^2(s\phi)\mathrm{d}\phi = \frac{1}{s}\int|\Phi_L|^2(s_3)\mathrm{d}s_3 = \frac{L}{s} \tag{12}$$

The function $B_{\pi/2}(s)$ is the integral width of the convolution in ϕ of $|\Phi_L|^2(s\phi)$ and $g_{\mathrm{eq}}(\phi)$. If $|\Phi_L|^2$ and g_{eq} can be approximated by Gaussian distributions, we obtain the relationship:

$$s^2B_{\pi/2}^{2}(s) = \frac{1}{L^2}+s^2B_{\Phi} \tag{13}$$

where $1/L$ and B_{eq} are the integral widths of $|\Phi_L|^2(s\phi)$ and $g_{\mathrm{eq}}(\phi)$, respectively.

Reference

[1] Thünemann A F, Ruland W. Microvoids in Polyacrylonitrile Fibers: A Small-Angle X-Ray Scattering Study[J]. Macromolecules, 2000, 33(5): 1848–1852.