On the Microstructure of High-Performance Polymer Materials

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Introduction

Due to the spinning process of many fibres, a nanoporous structure evolves inside the filaments. Investigations show a strong correlation between this nanoporous structure and the physical properties of the fibres. High-performance polymer fibres, such as aramid fibres (Twaron® and Kevlar®) show a similar nanoporous structure. Investigations with Small-Angle X-ray Scattering (SAXS) have the power of characterizing this structure, the results of which are invaluable in making structure-property relationships.

The SAXS methodology, however, may not be completely optimized for such systems of, what are assumed to be, cylindrical, aligned scatterers. These scatterers are nonuniform in shape, size and orientation, making them difficult to analyse.

This presentation focuses on the development of a validation method to test whether the obtained parameters from the analyses reflect the parameters of a true nanoporous system.

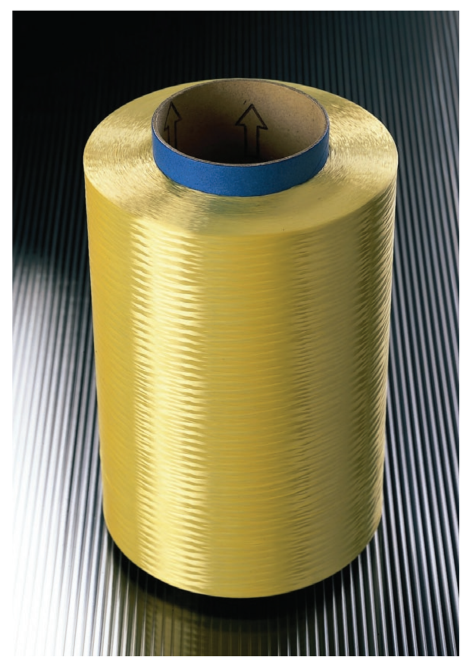


Figure 1: Twaron 1000. Image courtesy of Teijin Aramids

Validation method

Parameters

Parameters describing the orientation, size, length and position distribution are supplied as input

Simulation

A box is filled with cylinders or ellipsoids according to the supplied distributions. These make a 3D electron density grid.

Pattern

A discrete Fourier transform of the 3D grid forms a 3D intensity box. A cut through the box simulates a scattering pattern

Model Fit

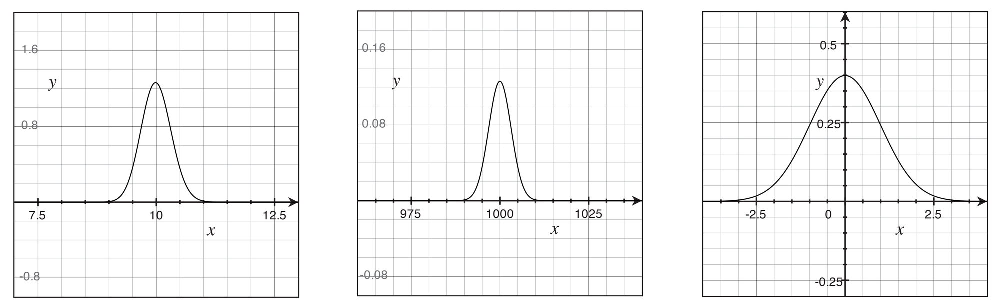
2D fits using standard models and newly developed models are let loose on the scattering patterns.

Parameters

Agreement between the thus obtained parameters and the starting values indicate the merit of each model.

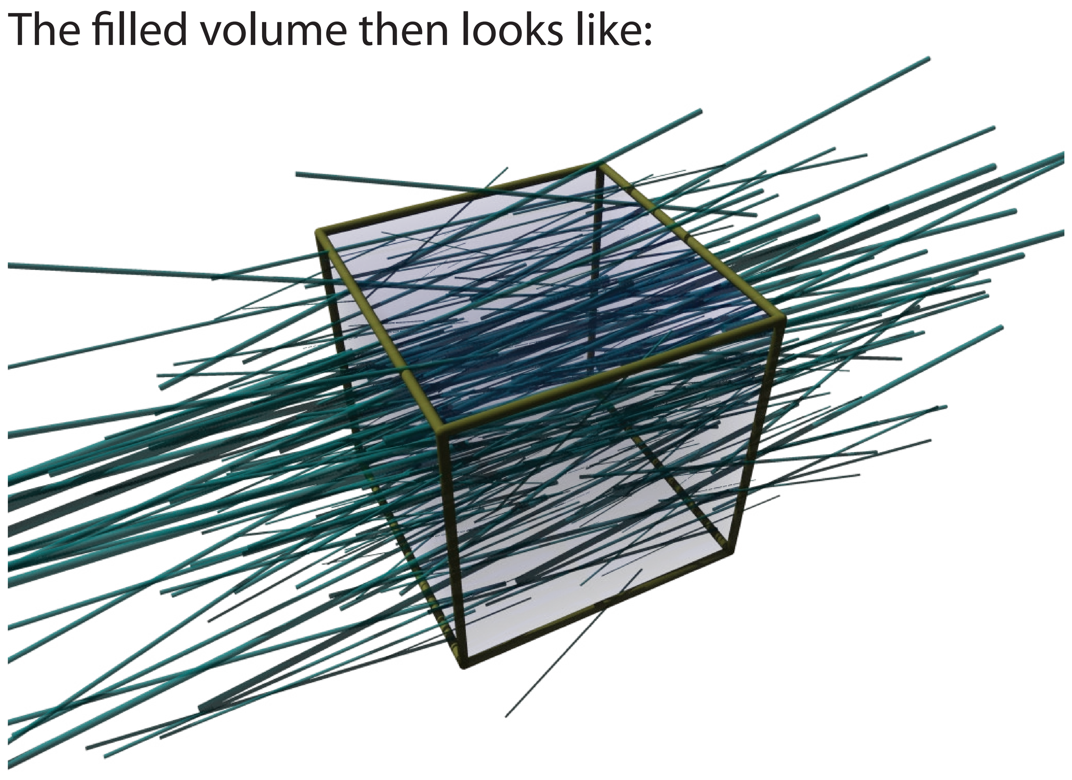
Progress

A simulated volume with sides of 2000 Ångströms is filled with enough cylinders to occupy a volume fraction of 1%. The cylinders have the following properties:



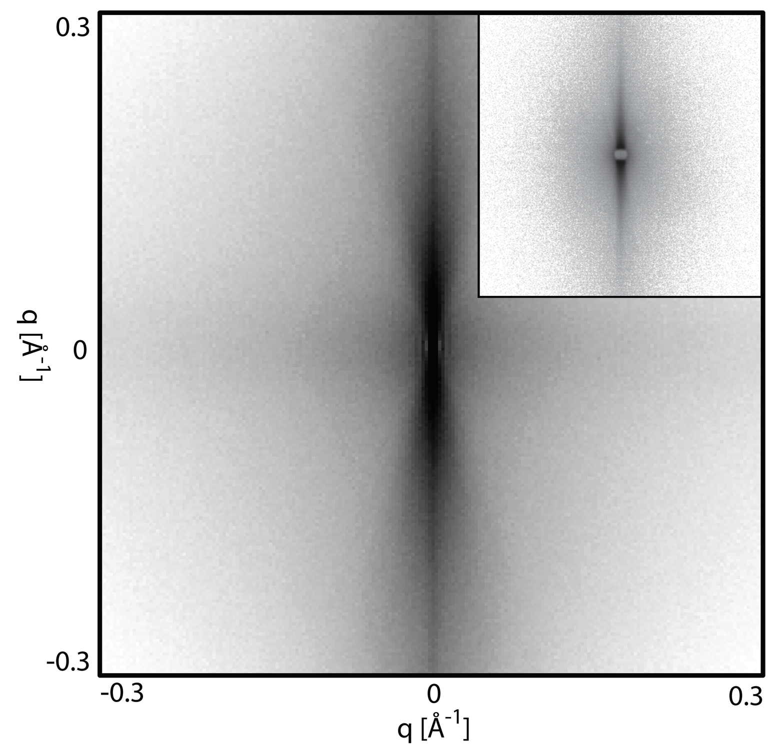
diameter [Å] | Height [Å] | Orientation [arcdegrees]

The filled volume then looks like:

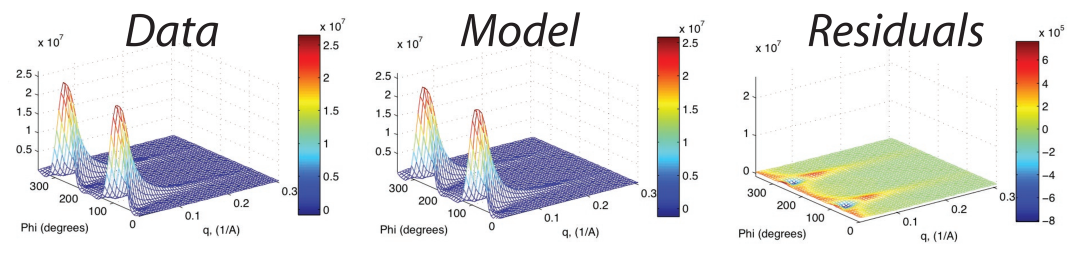


Where periodic boundary conditions apply. A grid is superimposed on the volume, and "voxels" (volume subdivisions) within a cylinder are marked. Thus, an electron density map is generated, which, after Discrete Fourier transformation, results in a 3D "scattered amplitude".

A 2D slice of the convoluted amplitude (i.e. the intensity), simulates the measured SAXS data (main), and resembles real Twaron SAXS data (inset):



The model fit of this simulated data (at first glance) appears quite well:



The fitted parameters, however, bear hardly any semblance to the original parameters, with:
- an orientation distribution width of 10 degrees,
- a height of 12.5 Å,
- and a diameter of 25 Å.

Conclusion

- Better fitting models must be developed
- More elementary simulations must be computed to determine the point of failure

Contextualization

The aspects of the project scope to which this topic applies: