

A Comprehensive Monte Carlo-Simulated Dataset of WAXD Patterns of Wood Cellulose Microfibrils

Ricardo Baettig ¹  and Ben Ingram ^{2*} 

¹ Facultad de Ciencias Forestales y de la Conservación de la Naturaleza, Universidad de Chile, La Pintana 8820808, Santiago, Chile; ricardo.baettig@uchile.cl

² Department of Interactive Visualization and Virtual Reality, Faculty of Engineering, Universidad de Talca, Talca 3460000, Talca, Chile

* Correspondence: bri@utalca.cl

Abstract: Wide-angle X-ray diffraction analysis is a powerful tool for investigating the structure and orientation of cellulose microfibrils in plant cell walls, but the complex relationship between diffraction patterns and underlying structural parameters remains challenging to both understand and validate. This study presents a comprehensive dataset of 81,906 Monte Carlo-simulated wide-angle X-ray diffraction patterns for the cellulose I β 200 lattice. The dataset was generated using a mechanistic, physically informed simulation procedure that incorporates realistic cell wall geometries from wood anatomy, including circular and polygonal fibers, and accounts for the full range of crystallographic and anatomical parameters influencing diffraction patterns. Each simulated pattern required multiple nested Monte Carlo iterations, totaling approximately 10 million calculations per pattern. The resulting dataset pairs each diffraction pattern with its exact generating parameter set, including mean microfibril angle (MFA), MFA variability, fiber tilt angles, and cell wall cross-sectional shape. The dataset addresses a significant barrier in the field—the lack of validated reference data with known ground truth values for testing and developing new analytical methods. It enables the development, validation, and benchmarking of novel algorithms and machine learning models for MFA prediction from diffraction patterns. The simulated data also allow for systematic investigation of the effects of geometric factors on diffraction patterns and serves as an educational resource for visualizing structure–diffraction relationships. Despite some limitations, such as assuming ideal diffraction conditions and focusing primarily on the S2 cell wall layer, this dataset provides a valuable foundation for advancing X-ray diffraction analysis methods for cellulose microfibril architecture characterization in plant cell walls.



check for updates

Academic Editor: Rüdiger Pryss

Received: 3 March 2025

Revised: 23 March 2025

Accepted: 27 March 2025

Published: 29 March 2025

Citation: Baettig, R.; Ingram, B. A Comprehensive Monte Carlo-Simulated Dataset of WAXD Patterns of Wood Cellulose Microfibrils. *Data* **2025**, *10*, 47. <https://doi.org/10.3390/data10040047>

Copyright: © 2025 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

Dataset: 10.6084/m9.figshare.28458716**Dataset License:** CC-BY 4.0

Keywords: cellulose microfibrils; microfibril angle; X-ray diffraction; wide-angle X-ray diffraction; Monte Carlo simulation; plant cell walls; wood anatomy; diffraction pattern analysis

1. Introduction

X-ray diffraction analysis has long been a powerful tool for investigating the structure and orientation of cellulose microfibrils in plant cell walls, with early studies dating back to the pioneering works of Sisson [1], Herzog and Jancke [2], Herzog et al. [3], and Preston [4]. As the most abundant biopolymer on Earth [5], cellulose has been a primary material for

industrial applications and energy production throughout history [6]. The advent of the 21st century bioeconomy has renewed interest in cellulose due to its potential for eco-friendly applications [7].

The stiffness of cellulose, with estimated tensile moduli ranging from 106 to 138 GPa [8–10], arises from its unique hierarchical structure. In vascular plants, cellulose I β microfibrils form helical structures around the cell wall, with their angular orientation relative to the cell axis defined as the microfibril angle (MFA) [11]. The MFA on the S2 cell wall layer is widely recognized as a critical determinant of the physical and mechanical properties of cellulosic materials, rivaling or even surpassing the importance of density [8,12].

Despite extensive research, the relationship between the MFA and the resulting X-ray diffraction patterns remains complex and challenging to validate [13–15]. The mathematical description of this relationship through the generalized cell wall tilt equation provides a physical basis for understanding diffraction patterns, but validating analytical methods has been limited by the lack of ground truth data, where the exact generating parameters are known. This dataset addresses this gap by providing simulated diffraction patterns with known parameters based on rigorous mathematical models. While both wide-angle X-ray diffraction (WAXD) and small-angle X-ray scattering (SAXS) are generally accepted methods for estimating the MFA [16], the literature often fails to clearly link MFA predictions to the anisotropic properties of plant fibers, such as shrinkage and mechanical characteristics [17].

This comprehensive dataset of simulated X-ray diffraction patterns addresses a critical gap in the field of plant cell wall analysis. Its unique value lies in providing researchers with a large collection of diffraction patterns paired with their exact generating parameters—a ground truth reference that is impossible to obtain through experimental methods alone [18,19]. By spanning the full parameter space of microfibril orientations, cross-sectional geometries, and fiber tilts, this dataset enables the development, validation, and benchmarking of new analytical algorithms and machine learning models for MFA prediction [15,20]. The applications of this resource extend beyond method development to educational purposes, allowing researchers to visualize the relationships between structural parameters and resulting diffraction patterns [21]. Furthermore, the dataset can serve as a testing ground for hypotheses regarding the impact of specific anatomical features on diffraction patterns without the need for specialized X-ray equipment [11,22]. The sharing of this computationally intensive simulation data aims to accelerate progress in understanding the cellulose architecture and its relationship to the mechanical properties of plant-based materials [12,23].

Over the past decade, theoretical advancements in WAXD-based MFA analysis have stagnated, with most studies relying on established methodologies despite their limitations [13,24,25]. The lack of a universally accepted method or gold standard for MFA prediction has led to challenges in validating results [26]. Discrepancies in the predictive capacity of MFA have been observed, with some studies reporting significant correlations with mechanical properties [23,27] and others finding inconclusive results [17,28,29].

These issues likely arise from the lack of procedures that account for cell-to-cell and within-cell wall variability of the MFA, cross-sectional shape, and fiber tilts [18]. The importance of accurately accounting for MFA variability within the cell wall has been highlighted by Cave and Robinson [18], who noted that a 5° change in MFA deviation can result in substantial errors in predicted values if not properly considered.

To address these challenges, this study presents a comprehensive dataset of 81,906 Monte Carlo-simulated X-ray diffraction patterns for the cellulose 200 lattice. This dataset, generated through physically informed simulations, incorporates cell wall geometries typical of wood anatomy and accounts for the full range of crystallographic and anatomical parameters influencing diffraction patterns. By providing a large-scale dataset with known

ground truth values for all geometric parameters, this research establishes a foundation for developing and validating improved methods for WAXD-based MFA analysis in plant cell walls. This dataset represents a significant step towards overcoming the lack of validated reference data, a major barrier in the field, and enables the development of more accurate and robust analytical techniques.

2. Data Description

The dataset presented in this study consists of two main components: simulated X-ray diffraction patterns and their associated generating parameters. These components are provided as separate CSV files, enabling researchers to easily access and analyze the data using a wide range of tools and programming environments.

2.1. Simulated Diffraction Patterns

The primary data file, *profiles*, contains the simulated X-ray diffraction patterns, where each row represents a complete 360° azimuthal intensity profile of the cellulose 200 lattice diffraction. The file structure comprises 361 columns: an *id* column that uniquely identifies each pattern and corresponds to the identifiers in the parameter file, followed by 360 columns (numbered 0–359) containing the intensity values at each azimuthal angle. Each column number corresponds directly to its azimuthal angle in degrees, providing a complete diffraction pattern with 1° angular resolution. These intensity profiles capture the characteristic double-peak pattern typically observed in cellulose 200 lattice diffraction, with peaks generally occurring around 90° and 270° for aligned samples, as shown in Figure 1.

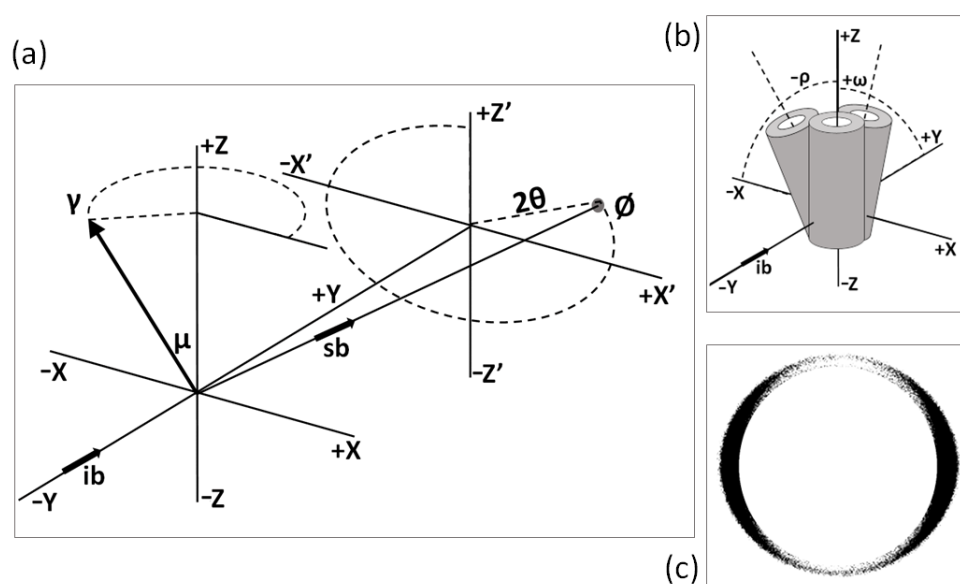


Figure 1. (a) The plot depicts the coordinate axes of the apparatus (shown in solid lines) along with the imaginary circles of the MFA spirals and diffraction spots (represented by dashed lines) according to the geometrical conditions for WAXD for cellulose 200 lattice. μ is the MFA, θ is the Bragg angle, γ is the angle of the cell wall tangent, and ϕ is the azimuthal angle where scattered beam *sb* hits the plane of detector *X'Z'* (*ib*: incident beam). (b) Misalignment (tilts) of fibers (ω and ρ) with respect to apparatus coordinates. (c) Typical 200 lattice diffraction pattern of unaltered cellulose-based fibers; intensity shows two opposite peaks.

The parameter file, *params*, contains the complete set of generating parameters for each diffraction pattern, as well as conventional analytical metrics calculated from the simulated profiles. This file includes the unique *id* column to link parameters with their

corresponding diffraction pattern, followed by columns for the generating parameters: cell wall cross-sectional shape template, mean MFA ($\bar{\mu}$), MFA standard deviation (σ_{μ}), mean fiber tilt angles ($\bar{\omega}$ and $\bar{\rho}$), tilt angle standard deviations (σ_{ω} and σ_{ρ}), and cell wall rotation angle (γ'). Table 1 provides a detailed description of the *params* data file structure.

Table 1. Parameters data file (*params*) structure.

Parameter	Col. Name	Type	Range	Description
Pattern ID	id	Integer	Variable	ID for diffraction pattern
Template	template	Integer	1–3	Cross-section shape type
$\bar{\mu}$	MFA	Float	$\mathcal{N}(25.0^{\circ}, 12.0^{\circ})$	Mean microfibril angle
σ_{μ}	desMFA	Float	$\mathcal{U}(5.0^{\circ}, 20.0^{\circ})$	MFA standard deviation
γ'	incl	Float	$\mathcal{N}(0.0^{\circ}, 10.0^{\circ})$	Template rotation angle
$\bar{\omega}$	omega	Float	$\mathcal{N}(0.0^{\circ}, 5.0^{\circ})$	Mean forward/backward tilt
σ_{ω}	desv_omega	Float	$\mathcal{U}(0.0^{\circ}, 5.0^{\circ})$	Forward/backward tilt standard deviation
$\bar{\rho}$	rho	Float	$\mathcal{N}(0^{\circ}, 5.0^{\circ})$	Mean lateral tilt
σ_{ρ}	desv_rho	Float	$\mathcal{U}(0^{\circ}, 5.0^{\circ})$	Lateral tilt standard deviation
VA MFA (Peak 1)	VA_MFA1	Float	Variable	Variance approach MFA estimate for first peak
VA MFA (Peak 2)	VA_MFA2	Float	Variable	Variance approach MFA estimate for second peak
Peak 1 Std Dev	desv1	Float	Variable	Standard deviation of first diffraction peak
Peak 2 Std Dev	desv2	Float	Variable	Standard deviation of second diffraction peak
Peak 1 Variance	var1	Float	Variable	Variance of first diffraction peak
Peak 2 Variance	var2	Float	Variable	Variance of second diffraction peak

The inclusion of these stochastic parameters allows for a comprehensive analysis of how diffraction patterns vary with changes in structural and geometric factors. Cell wall shapes were selected based on anatomical patterns observed in wood, covering circular fibers typical of hardwood and reaction wood [30] as well as polygonal tracheids characteristic of normal softwood [31,32]. By incorporating realistic cell wall geometries and their variability, this dataset captures the complexity of wood cell wall structures in simulated diffraction patterns [33,34].

The parameter file also includes conventional analytical metrics calculated from the simulated diffraction patterns using established methods. These include the T parameter [13,24] and the variance approach [25,35]. The inclusion of these metrics allows for direct comparison between simulated patterns and traditional WAXD analyses, facilitating the validation of existing methods and the development of new analytical approaches [36–38].

All intensity values in the *profiles* file are normalized and represent relative diffraction intensities. The azimuthal profiles are recorded without integration in the 2θ direction, simulating diffraction patterns at constant momentum transfer corresponding to the cellulose 200 lattice peak. Table 2 summarizes the structure of the *profiles* data file.

Table 2. Diffraction pattern data file (*profiles*) structure.

Parameter	Column Name	Type	Range	Description
Pattern ID	id	Integer	Variable	ID for diffraction pattern
Intensity Vector	0.. 359	Float Array	[0, max]	360° azimuthal intensity profile

2.2. Cell Wall Templates

Three template files defining cross-sectional shapes are used in the simulations, as shown in Figure 2.

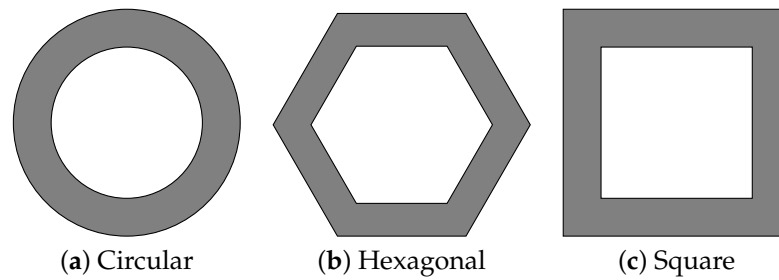


Figure 2. The three cross-section templates shown here were used as base models: (a) Circular, (b) hexagonal, and (c) square. For each diffraction pattern generated in the 81,906-pattern dataset, one of these templates was randomly selected.

3. Methods

3.1. Dataset Generation

The dataset was generated using a Monte Carlo simulation procedure based on established WAXD physics. The foundation of this simulation is the generalized tilt equation (Equation (1)) that describes the 200 lattice diffraction condition for cellulose microfibrils with various orientations and tilts:

$$\pm \{ \sin(\phi - \omega) \cos(\theta) \sin(\mu) \cos(\gamma) - \sin(\theta) [\cos(\rho) \sin(\gamma) \sin(\mu) - \sin(\rho) \cos(\mu)] + \cos(\theta) \cos(\phi - \omega) [\sin(\rho) \sin(\mu) \sin(\gamma) + \cos(\rho) \cos(\mu)] \} = 0 \quad (1)$$

In this equation, θ represents the Bragg angle, μ is the microfibril angle, γ is the angle of the cell wall tangent, ϕ is the azimuthal angle where the scattered beam hits the detector plane, and ω and ρ represent the tilts of the fiber with respect to apparatus coordinates (forward/backward and lateral tilts, respectively).

For the generation of diffraction patterns, the solutions for ϕ in Equation (1) are calculated using

$$\phi = \tan^{-1} \left(\frac{B}{A} \right) \pm \cos^{-1} \left(\frac{C}{\sqrt{A^2 + B^2}} \right) + m\pi + \omega \quad (2)$$

where the components are defined as

$$A = \cos(\theta) \sin(\rho) \sin(\mu) \sin(\gamma) + \cos(\theta) \cos(\rho) \cos(\mu) \quad (3)$$

$$B = \cos(\theta) \sin(\mu) \cos(\gamma) \quad (4)$$

$$C = \sin(\theta) \cos(\rho) \sin(\mu) \sin(\gamma) - \sin(\theta) \sin(\rho) \cos(\mu) \quad (5)$$

$$m = \begin{cases} 1, & A > 0 \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

Using these equations, each diffraction pattern in the dataset was generated through a multi-step Monte Carlo simulation procedure, as shown in Figure 3.

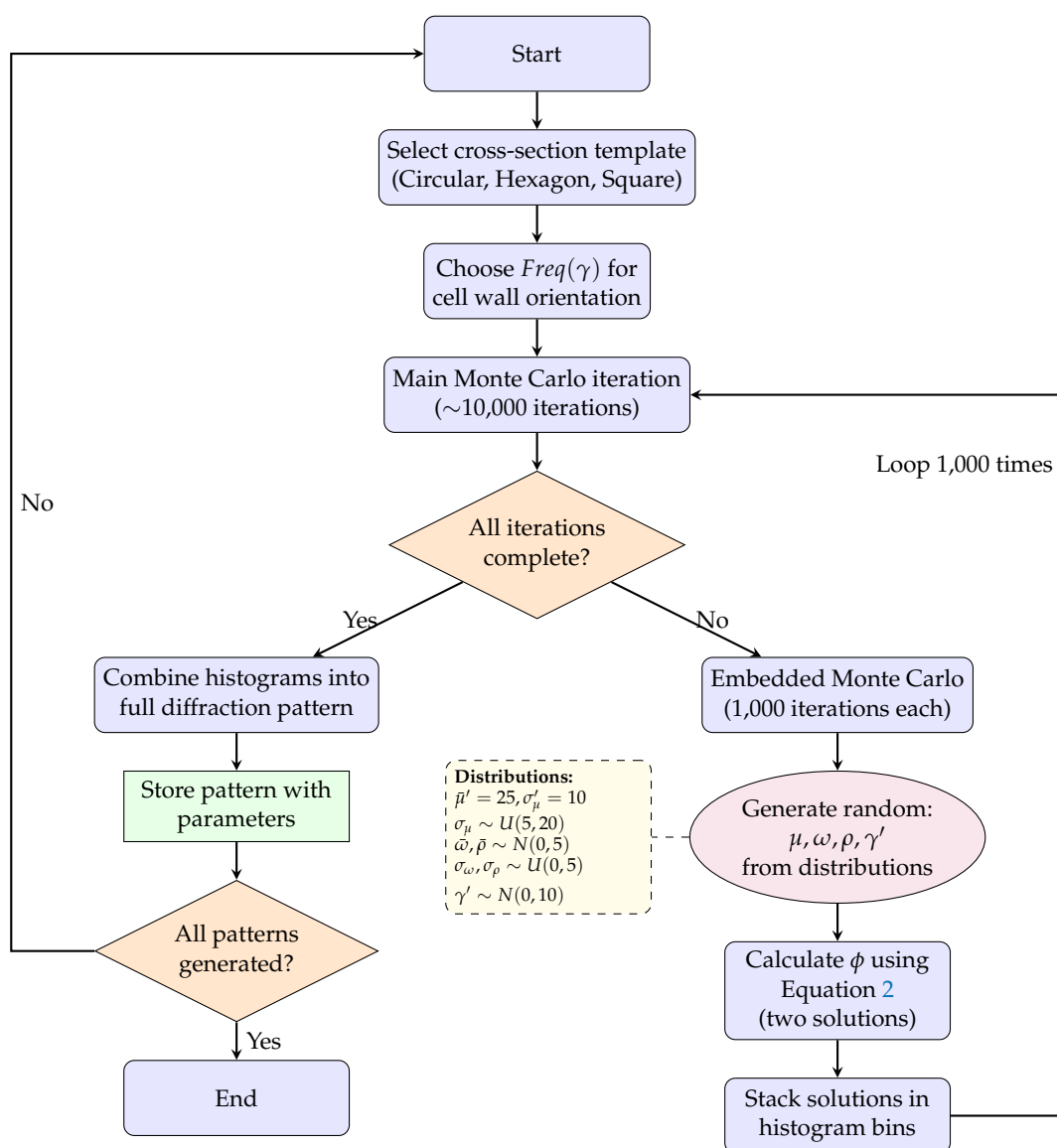


Figure 3. Flowchart of the Monte Carlo simulation procedure used to generate the diffraction pattern dataset. The nested loop structure shows how each of the 10,000 main iterations contains 1000 embedded iterations, resulting in approximately 10 million calculations per diffraction pattern.

3.2. Validation

The validation of the simulated dataset was conducted through a twofold approach. First, the generated diffraction patterns were compared against experimental X-ray diffraction data to ensure that the simulations accurately captured the key features and characteristics of real-world measurements. This comparison provided a qualitative assessment of the dataset's fidelity to physical reality. Second, a thorough analysis of the parameter distributions and correlations within the dataset was performed. This quantitative evaluation verified that the simulated data exhibited realistic distributions and relationships between the various structural and geometric parameters, consistent with the expected behavior based on the underlying physics and wood anatomy.

4. User Notes

4.1. Data Format

The simulated X-ray diffraction dataset is provided in a standard comma-separated value (CSV) format, ensuring compatibility with a wide range of data analysis tools and

programming environments. Each row in the dataset represents a single diffraction pattern, with columns corresponding to the azimuthal intensity values (0 through 359) and the associated geometric parameters (template, $\bar{\mu}$, σ_{μ} , $\bar{\omega}$, σ_{ω} , $\bar{\rho}$, σ_{ρ} , γ'). The azimuthal intensity values capture the complete 360° diffraction profile with a 1° angular resolution, enabling detailed analysis of the diffraction patterns.

Figure 4 demonstrates the fidelity of our simulation approach by comparing real-world experimental diffraction patterns with their most similar simulated counterparts; Tables 3–5 show the generating parameters for each of the profiles in the plot. The close correspondence between measured and simulated patterns illustrates the representativeness and realistic nature of the simulated data, validating its utility for training accurate predictive models of wood microstructure.

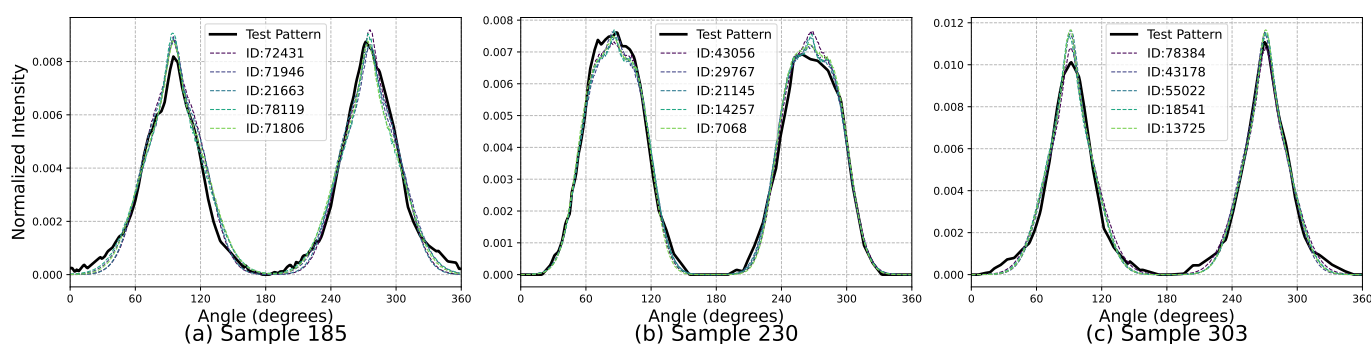


Figure 4. Plot of sample profiles and 5 nearest simulated profiles. (a) Sample 185, (b) Sample 230, and (c) Sample 303.

Table 3. Sample 185 and 5 nearest simulated profiles with generating MFA and desMFA (Figure 4a).

ID	MFA	desMFA
72431	26.8°	15.3°
71946	28.0°	17.6°
21663	27.5°	14.9°
78119	27.8°	18.8°
71806	28.2°	16.8°

Table 4. Sample 230 and 5 nearest simulated profiles with generating MFA and desMFA (Figure 4b).

ID	MFA	desMFA
43056	27.7°	12.6°
29767	28.1°	12.9°
21145	28.3°	13.2°
14257	28.1°	12.9°
7068	27.9°	11.8°

Table 5. Sample 303 and 5 nearest simulated profiles with generating MFA and desMFA (Figure 4c).

ID	MFA	desMFA
78384	22.9°	16.1°
43178	22.0°	14.0°
55022	21.5°	14.8°
18541	22.0°	14.5°
13725	22.1°	14.5°

The data also include asymmetric diffraction patterns, as shown in Figure 5, which arise from lateral tilts ($\bar{\rho}$) causing the 200 lattice peaks to deviate from their idealized 180°

opposition. These asymmetric patterns are commonly observed in real-world samples where cell wall segments fail to align symmetrically with the incident X-ray beam due to natural growth variations or specimen preparation artifacts. Our simulation framework incorporates these tilts through the generalized diffraction equation (Equation (1)), ensuring that the trained models can accurately interpret the full spectrum of diffraction patterns encountered in experimental settings.

To further explore the simulated profiles, the Supplementary Materials include a link to a video where each profile is plotted, with the associated generating parameters.

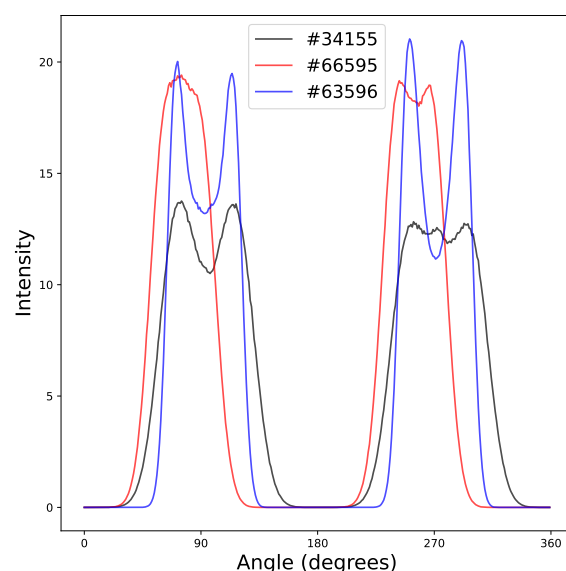


Figure 5. Plot of three randomly selected asymmetric profiles.

4.2. Recommended Applications

The comprehensive nature of this simulated dataset makes it particularly suitable for a range of applications in the field of X-ray diffraction analysis of cellulose microfibrils. One key application is the development and validation of new methods for predicting the microfibril angle (MFA) from diffraction patterns. The dataset's large size and known ground truth values for MFA and other parameters provide an ideal testbed for evaluating the accuracy and robustness of novel prediction algorithms. Additionally, the dataset is well suited for training and validation of machine learning models, which can leverage the rich parameter space to learn complex relationships between diffraction patterns and underlying structural features. The simulated data also enable systematic investigation of the effects of various geometric factors, such as cell wall cross-sectional shape and fiber tilts, on the resulting diffraction patterns. This can provide valuable insights into the sensitivity of diffraction methods to these parameters and guide the interpretation of experimental data. Finally, the dataset serves as a benchmark for comparing and assessing the performance of existing and future prediction algorithms, promoting standardization and reproducibility in the field.

4.3. Assumptions and Considerations

Researchers working with this dataset should note that the simulated diffraction patterns were generated with specific assumptions about the X-ray beam geometry and specimen characteristics. Users seeking to compare these simulations with experimental data should ensure their experimental setup aligns with these assumptions or apply appropriate corrections for different geometries. Additionally, when analyzing the patterns, researchers should be aware that the intensity values are normalized and do not reflect

absolute scattering intensities; comparisons between patterns should focus on relative intensity distributions rather than absolute values.

The background effect in the diffraction patterns, which arises from amorphous molecules and the S1, S3, and P layers of the cell wall, was not considered in the simulations. This simplification is reasonable, as in empirical patterns the baseline is typically eliminated prior to analysis. However, researchers should be aware of this assumption when comparing simulated data to experimental results and account for any potential discrepancies introduced by the presence of background signal in real-world measurements.

4.4. Data Subsetting and Filtering

Efficient use of this large dataset can be facilitated by initially subsetting the data based on specific parameter ranges of interest. For example, researchers focusing on compression wood might prioritize patterns with high MFA values ($>30^\circ$), while those interested in tension wood or normal wood might focus on lower MFA ranges. The dataset can be easily filtered using common data analysis tools such as Python with pandas [39,40], R [41], or specialized scientific software.

4.5. Analytical Method Development

Development of new analytical methods benefits from a training–validation–test approach, where model development occurs on a subset of the data, with final validation performed on a separate holdout set to ensure generalizability [42]. Visualization of the relationship between input parameters and resulting diffraction patterns through dimensionality reduction techniques such as PCA [43] or t-SNE [44] can reveal clusters and trends within the parameter space.

4.6. Machine Learning Applications

For machine learning applications, the dataset has been intentionally structured to support both supervised learning (predicting parameters from patterns) and unsupervised approaches (discovering inherent structure in the diffraction patterns) [45,46]. Various feature extraction methods warrant consideration, as the raw 360-point intensity profiles may benefit from preprocessing such as smoothing, peak detection [47], or transformation to frequency domain representations. When comparing prediction accuracies, metrics that account for the circular nature of angular data, such as circular mean absolute error or angular correlation coefficients [48,49], are preferable to standard regression metrics.

4.7. Limitations

While the simulated dataset offers a valuable resource for X-ray diffraction analysis of cellulose microfibrils, users should be aware of certain limitations. The simulated data assume ideal diffraction conditions, which may not fully capture the complexities and variability encountered in real-world experiments. Additionally, the dataset is limited to three basic cross-sectional templates (circular, hexagonal, and square), which, although representative of common wood cell geometries, may not encompass the full diversity of cell wall shapes found in nature. The simulations also do not account for the effects of the S1 and S3 layers of the cell wall, focusing primarily on the S2 layer, which is the main contributor to the diffraction signal. Lastly, the dataset assumes a constant momentum transfer, meaning that the intensity values are recorded without integration in the 2θ direction. While this simplification is common in the analysis of the cellulose 200 peak, it may limit the direct comparability to experimental data that integrate over a range of 2θ values. Despite these limitations, the simulated dataset provides a valuable starting point for understanding the complex relationships between cellulose microfibril structure and X-ray diffraction patterns, and serves as a foundation for future research and method development in this field.

Supplementary Materials: A video of all simulated profiles with generating parameters is available at: <http://www.doi.org/10.6084/m9.figshare.28644365> (accessed on 28 March 2025).

Author Contributions: Conceptualization, R.B.; methodology, R.B. and B.I.; software, R.B. and B.I.; validation, R.B. and B.I.; investigation, R.B. and B.I.; resources, R.B. and B.I.; data curation, R.B. and B.I.; writing—original draft preparation, R.B. and B.I.; writing—review and editing, R.B. and B.I.; visualization, R.B. and B.I. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data available at: <https://doi.org/10.6084/m9.figshare.28458716> (accessed on 28 March 2025).

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Sisson, W. X-Ray Studies of Crystallite Orientation in Cellulose Fibers. *Ind. Eng. Chem.* **1935**, *27*, 51–56.
2. Herzog, R.; Jancke, W. Röntgenspektrographische Beobachtungen an Zellulose. *Z. Für Phys.* **1920**, *3*, 196–198.
3. Herzog, R.; Jancke, W.; Polanyi, M. Röntgenspektrographische Beobachtungen an Zellulose. II. *Z. Für Phys.* **1920**, *3*, 343–348.
4. Preston, R. The fine structure of the wall of the conifer tracheid I. The X-ray diagram of conifer wood. *Proc. R. Soc. Lond. Ser. B-Biol. Sci.* **1946**, *133*, 327–348.
5. Li, T.; Chen, C.; Brozena, A.; Zu, J. Developing fibrillated cellulose as a sustainable technological material. *Nature* **2021**, *590*, 47–56. [[PubMed](#)]
6. Hall, J. Wood in an industrial world. *Sci. Mon.* **1948**, *27*, 398–405.
7. Wang, J.; Wang, L.; Gardner, D.; Shaler, S.M.; Cai, Z. Towards a cellulose-based society: Opportunities and challenges. *Cellulose* **2021**, *28*, 4511–4543. [[CrossRef](#)]
8. Sakurada, I.; Nukushina, Y.; Ito, T. Experimental determination of the elastic modulus of crystalline regions in oriented polymers. *J. Polym. Sci.* **1962**, *57*, 651–660.
9. Matsuo, M.; Sawatari, C.; Iwai, Y.; Ozaki, F. Effect of Orientation Distribution and Crystallinity on the Measurement by X-ray Diffraction of the Crystal Lattice Moduli of Cellulose I and II. *Macromolecules* **1990**, *23*, 3266–3275.
10. Nishino, T.; Takano, K.; Nakamae, K. Elastic modulus of the crystalline regions of cellulose polymorphs. *J. Polym. Sci. Part B Polym. Phys.* **1995**, *33*, 1647–1651.
11. Rongpipi, S.; Ye, D.; Gomez, E.; Gomez, E. Progress and Opportunities in the Characterization of Cellulose—An Important Regulator of Cell Wall Growth and Mechanics. *Front. Plant Sci.* **2019**, *9*, 1894. [[CrossRef](#)]
12. Salmén, L. Micromechanical understanding of the cell-wall structure. *C. R. Biol.* **2004**, *327*, 873–880. [[CrossRef](#)]
13. Cave, I. Theory of X-ray Measurement of Microfibril Angle in Wood. *For. Prod. J.* **1966**, *16*, 37–42.
14. Yamamoto, H.; Okuyama, T.; Yoshida, M. Method of Determining the Mean Microfibril Angle of Wood Over a Wide Range by the Improved Cave's Method. *Mokuzai Gakkaishi* **1993**, *39*, 375–381.
15. Verrill, S.; Kretschmann, D.; Herian, V.; Wiemann, M.; Alden, H. Concerns about a variance approach to X-ray diffractometric estimation of microfibril angle in wood. *Wood Fiber Sci.* **2011**, *43*, 153–168.
16. Lichtenegger, H.; Reiterer, A.; Stanzl-Tschegg, S.; Fratzl, P. Comment about “The measurement of the micro-fibril angle in soft-wood” by K. M. Entwistle and N. J. Terrill. *J. Mater. Sci. Lett.* **2001**, *20*, 2245–2247.
17. Wang, X.; Ma, J.; Xu, W.; Fei, B.; Lian, C.; Sun, F. Effect of bending on radial distribution density, MFA and MOE of bent bamboo. *Sci. Rep.* **2022**, *12*, 8610. [[CrossRef](#)]
18. Cave, I.; Robinson, W. Interpretation of (002) diffraction arcs by means of a minimalist model. In *Microfibril Angle in Wood*; Butterfield, B.G., Ed.; Proceedings of the IAWA/IUFRO International Workshop on the Significance of Microfibril Angle to Wood Quality; University of Canterbury Press: Westport, New Zealand, 1997.
19. Lichtenegger, H.; Müller, M.; Wimmer, R.; Fratzl, P. Microfibril Angles Inside and Outside Crossfields of Norway Spruce Tracheids. *Holzforschung* **2003**, *57*, 13–20.
20. Kobayashi, K.; Hwang, S.W.; Okochi, T.; Lee, W.H.; Sugiyama, J. Non-destructive method for wood identification using conventional X-ray computed tomography data. *J. Cult. Herit.* **2019**, *38*, 88–93. [[CrossRef](#)]
21. Donaldson, L.A. Wood cell wall ultrastructure the key to understanding wood properties and behaviour. *IAWA J.* **2019**, *40*, 645–672.

22. Keplinger, T.; Wang, X.; Burgert, I. Nanofibrillated cellulose composites and wood derived scaffolds for functional materials. *J. Mater. Chem. A* **2019**, *7*, 2981–2992. [\[CrossRef\]](#)
23. Yang, J.; Evans, R. Prediction of MOE of eucalypt wood from microfibril angle and density. *Holz Als Roh- Und Werkst.* **2003**, *61*, 449–452. [\[CrossRef\]](#)
24. Meylan, B. Measurement of Microfibril Angle by X-Ray Diffraction. *For. Prod. J.* **1967**, *17*, 51–58.
25. Evans, R. A variance approach to the X-ray diffractometric estimation of microfibril angle in wood. *Appita J.* **1999**, *52*, 283–289.
26. Evans, R. Rapid scanning of microfibril angle in increment cores by X-ray diffractometry. In *Microfibril Angle in Wood*; Butterfield, B.G., Ed.; Proceedings of the IAWA/IUFRO International Workshop on the Significance of Microfibril Angle to Wood Quality; University of Canterbury Press: Westport, New Zealand, 1997.
27. Eder, M.; Arnould, O.; William, J.; Dunlop, C.; Hornatowska, J.; Salmén, L. Experimental micromechanical characterisation of wood cell walls. *Wood Sci. Technol.* **2013**, *45*, 461–472. [\[CrossRef\]](#)
28. Hein, P.; Lima, J. Relationships between microfibril angle, modulus of elasticity and compressive strength in Eucalyptus wood. *Maderas. Cienc. Y Tecnol.* **2012**, *14*, 267–274.
29. Hein, P.; Lima, J.; Brancheriau, L. Correlations among microfibril angle, density, modulus of elasticity, modulus of rupture and shrinkage in 6-year-old Eucalyptus urophylla × E. grandis. *Maderas. Cienc. Y Tecnol.* **2013**, *15*, 171–182.
30. Donaldson, L.; Singh, A. Formation and Structure of Compression Wood. In *Cellular Aspects of Wood Formation*; Fromm, J., Ed.; Springer-Verlag: Berlin/Heidelberg, Germany, 2013; pp. 225–256.
31. Watanabe, U.; Norimoto, M.; Fujita, M.; Gril, J. Structural Variation of Tracheids in Norway Spruce (*Picea abies* [L.] Karst.). *J. Wood Sci.* **1998**, *44*, 9–14. [\[CrossRef\]](#)
32. Sarén, M.; Serimaa, R.; Andersson, S.; Paakkari, T.; Saranpää, P.; Pesonen, E. Transverse shrinkage anisotropy of coniferous wood investigated by the power spectrum analysis. *J. Struct. Biol.* **2001**, *136*, 101–109. [\[CrossRef\]](#)
33. Anagnost, S.; Mark, R.; Hanna, R. Variation of microfibril angle within individual tracheids. *Wood Fiber Sci.* **2002**, *34*, 377–349.
34. Lichtenegger, H.; Reiterer, A.; Stanzl-Tschegg, S.; Fratzl, P. Variation of Cellulose Microfibril Angles in Softwoods and Hardwoods—A Possible Strategy of Mechanical Optimization. *J. Struct. Biol.* **1999**, *128*, 257–269.
35. Evans, R.; Hughes, M.; Menz, D. Microfibril angle variation by scanning X-ray diffractometry. *Appita J.* **1999**, *52*, 363–367.
36. Verrill, S.; Kretschmann, D.; Herian, V. JMFA—A Graphically Interactive Java Program that Fits Microfibril Angle X-ray Diffraction Data. In *Res. Note FPL-RN-0283*; U.S. Department of Agriculture, Forest Service, Forest Products Laboratory: Madison, WI, USA, 2001.
37. Verrill, S.; Kretschmann, D.; Herian, V. JMFA 2—A Graphically Interactive Java Program that Fits Microfibril Angle X-ray Diffraction Data. In *Res. Note FPL-RP-635*; U.S. Department of Agriculture, Forest Service, Forest Products Laboratory: Madison, WI, USA, 2006.
38. Sarén, M.; Serimaa, R. Determination of microfibril angle distribution by X-ray diffraction. *Wood Sci. Technol.* **2006**, *40*, 445–460.
39. McKinney, W. Data structures for statistical computing in Python. *SciPy* **2010**, *445*, 51–56.
40. Van Der Walt, S.; Colbert, S.C.; Varoquaux, G. The NumPy array: A structure for efficient numerical computation. *Comput. Sci. Eng.* **2011**, *13*, 22–30. [\[CrossRef\]](#)
41. R Core Team. *R: A Language and Environment for Statistical Computing*; R Foundation for Statistical Computing: Vienna, Austria, 2023.
42. Hastie, T.; Tibshirani, R.; Friedman, J. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*, 2nd ed.; Springer Science & Business Media: Berlin/Heidelberg, Germany, 2009.
43. Abdi, H.; Williams, L.J. Principal component analysis. *Wiley Interdiscip. Rev. Comput. Stat.* **2010**, *2*, 433–459.
44. Maaten, L.v.d.; Hinton, G. Visualizing data using t-SNE. *J. Mach. Learn. Res.* **2008**, *9*, 2579–2605.
45. Jordan, M.I.; Mitchell, T.M. Machine learning: Trends, perspectives, and prospects. *Science* **2015**, *349*, 255–260.
46. LeCun, Y.; Bengio, Y.; Hinton, G. Deep learning. *Nature* **2015**, *521*, 436–444.
47. Virtanen, P.; Gommers, R.; Oliphant, T.E.; Haberland, M.; Reddy, T.; Cournapeau, D.; Burovski, E.; Peterson, P.; Weckesser, W.; Bright, J.; et al. SciPy 1.0: Fundamental algorithms for scientific computing in Python. *Nat. Methods* **2020**, *17*, 261–272.
48. Berens, P. CircStat: A MATLAB toolbox for circular statistics. *J. Stat. Softw.* **2009**, *31*, 1–21. [\[CrossRef\]](#)
49. Mardia, K.V.; Jupp, P.E. *Directional Statistics*; John Wiley & Sons: Chichester, UK, 2000.

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.