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Characterization of BF leaf powder by X-Ray diffraction

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Abstract

The Palmyra palm (*Borassus flabellifer*), a multipurpose tree of great utility It is cultivated in many tropical areas for its leaf, fruit, sap and many other items. The fibre obtained from the base of the petioles, or the sheathing leafstalks, is stiff, harsh and wiry. X-ray diffraction has been a well-established technique in the field of structural investigations for decades, applied not only by physicists. It represents an important tool for Physicists, chemists and biologists, too, and played a decisive role in the discovery of the structure material. Crystallography can reliably provide the answer to many structures related questions, from global folds to atomic details of bonding. The *Borassus flabellifer* leaves could be considered as good sources of natural antioxidants and antimicrobials and may find several applications in agro-food and pharmaceutical industries. The present work will help tribal of Madhya Pradesh for upgrading their Social and economic condition.

Keywords: interference, diffraction, amplitude, monochromatic

1. Introduction

The Palmyra palm (*Borassus flabellifer*), a multipurpose tree of great utility, occurs extensively in Tamil Nadu state, India. *Borassus flabellifer* Increasing exploitation of the Palmyra threatens the future supply of palm raw materials so important to rural populations. Integrated development of Palmyra products for local and export markets, as well as management/conservation measures, are needed both to maximize the economic value of the products and to assure sustained yield from native stands. The Palmyra palm is a very tall, single-stemmed evergreen palm tree that can eventually reach a height of 30 meters. The unbranched stem can be up to 1 meter wide at the base, narrowing to 40 - 50cm at around 4 meters and thereafter cylindrical; it is topped by a crown of up to 60 large, stiffly projecting fan-shaped-leaves. The tree is widely exploited in areas where it grows and has a very wide range of applications. Indeed, in India it is called the tree with 800 uses. It is cultivated in many tropical areas for its leaf, fruit, sap and many other items. It is one of the most important of the cultivated palms, though it is falling out of favour because of the long time taken to bring a crop from seed to maturity (12 years or more). Nowadays it is mainly cultivated in the drier parts of its geographical range. A number of different fibres can be obtained from the plant. A fibre obtained from the leaves is used to make string, rope, fencing etc. The fibres of young leaves can be woven into delicate patterns. The fibre obtained from the base of the petioles, or the sheathing leafstalks, is stiff, harsh and wiry. It is used to make brushes etc. Petioles are often can be split into fibre, to be used for weaving and matting. A fibre is obtained from the inner bark. The bark fibre can be used to make strong ropes. The *Borassus flabellifer* leaves are used for thatching, mats, baskets, fans, hats, umbrellas, and as writing material. The skin of the stem can be peeled off and be used as rope and also used to weave into cots (நாற்கட்டி in Tamil). In some part of Tamil Nadu, a variety of rice flour cake (called "Kolukattai") is prepared using the leaf. In the eastern part of India, the leaves are used to make hand fans. These are mostly used during the summer in parts of Assam and West Bengal. The *Borassus flabellifer* leaves could be considered as good sources of natural antioxidants and antimicrobials and may find several applications in agro-food and pharmaceutical industries.

X-ray diffraction has been a well-established technique in the field of structural investigations for decades, applied not only by physicists. It represents an important tool for

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Physicists, chemists and biologists, too, played a decisive role in the discovery of the structure material. Any method that exploits X rays is based upon their discovery in 1895 by W. C. Röntgen by chance while studying the charge transport in gases. This achievement was rewarded the first Nobel prize in the field of physics ever, in 1901. The first diffraction experiment was performed by Max v. Laue in 1912 observed diffraction pattern. With this single photograph, Laue solved at once two major problems of his days: It clearly reveals the crystalline nature of solids and proves that X rays behave like waves. This finding was rewarded the Nobel Prize in 1914. Since x-ray diffraction is a rather old technique. X-ray crystallography is an experimental technique that exploits the fact that X-rays are diffracted by crystals. It is not an imaging technique. X-rays have the proper wavelength (i th in the Ångström range, $\sim 10^{-10}$ m) to be scattered by the electron cloud of an atom of comparable size. Based on the diffraction pattern obtained from X-ray scattering off the periodic assembly of molecules or atoms in the crystal, the electron density can be reconstructed. Additional phase information must be extracted either from the diffraction data or from supplementing diffraction experiments to complete the reconstruction. The knowledge of accurate molecular structures is a prerequisite for rational drug design and for structure based functional studies to aid the development of effective therapeutic agents and drugs. Crystallography can reliably provide the answer to many structures related questions, from global folds to atomic details of bonding. The target material of the X-ray tube is bombarded with electrons accelerated from the cathode filament, two types of X-ray spectra are produced. The first is called the continuous spectra. The continuous spectrum consists of a range of wavelengths of X-rays with minimum wavelength and intensity (measured in counts per second) dependent on the target material and the Voltage across the X-ray tube. The minimum wavelength decreases and the intensity increases as voltage increases. The second type of spectra, called the *characteristic spectra*, is produced at high voltage as a result of specific electronic transitions that take place within individual atoms of the target material.

2. Method

A beam of X-rays consists of a bundle of separate waves, the waves can interact with one another. Such interaction is

termed *interference*. If all the waves in the bundle are in phase, that is their crests and troughs occur at exactly the same position (the same as being an integer number of wavelengths out of phase, $n\lambda$, $n = 1, 2, 3, 4$, etc.), the waves will interfere with one another and their amplitudes will add together to produce a resultant wave that is has a higher amplitude (the sum of all the waves that are in phase. If the waves are out of phase, being off by a non-integer number of wavelengths, then destructive interference will occur and the amplitude of the waves will be reduced. In an extreme case, if the waves are out of phase by an odd multiple of $1/2\lambda$ [$(2n+1)/2\lambda$], the resultant wave will have no amplitude and thus be completely destroyed. The atoms in crystals interact with X-ray waves in such a way as to produce interference. The interaction can be thought of as if the atoms in a crystal structure reflect the waves. But, because a crystal structure consists of an orderly arrangement of atoms, the reflections occur from what appears to be planes of atoms. Let's imagine a beam of X-rays entering a crystal with one of these planes of atoms oriented at an angle of θ to the incoming beam of monochromatic X-rays (monochromatic means one color, or in this case 1 discrete wavelength as produced by the characteristic spectra of the X-ray tube). Two such X-rays are shown here, where the spacing between the atomic planes occurs over the distance, d . Ray 1 reflects off of the upper atomic plane at an angle θ equal to its angle of incidence. Similarly, Ray 2 reflects off the lower atomic plane at the same angle θ . While Ray 2 is in the crystal, however, it travels a distance of $2a$ farther than Ray 1. If this distance $2a$ is equal to an integral number of wavelengths ($n\lambda$), then Rays 1 and 2 will be in phase on their exit from the crystal and constructive interference will occur. If the distance $2a$ is not an integral number of wavelengths, then destructive interference will occur and the waves will not be as strong as when they entered the crystal. Thus, the condition for constructive interference to occur is $n\lambda = 2a$ but, from trigonometry, we can figure out what the distance $2a$ is in terms of the spacing, d , between the atomic planes. To measure two theta, we used SHIMADZU XRD-7000 X-ray diffraction meter.

$$a = d \sin \theta; \text{ or } 2a = 2 d \sin \theta;$$

$$\text{Thus, } n\lambda = 2d \sin \theta$$

This is known as Bragg's Law for X-ray diffraction.

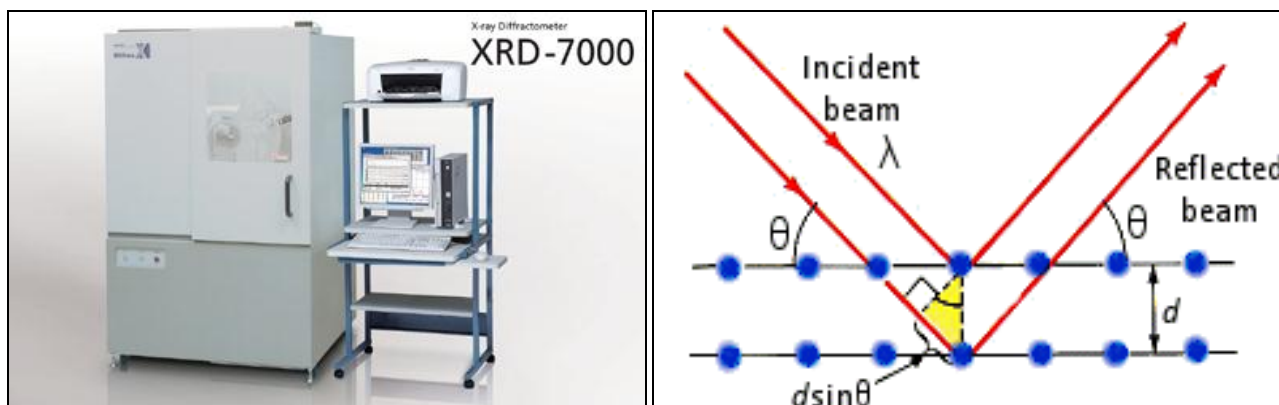


Fig 1: Instrument used to measure diffraction of X-rays

3. Result

The X-ray diffraction result of Borassus flabellifer as follows:-

File Name: BF-Leaf Powder -male PKR

Peak Data file

comment = BF-Leaf Powder-male
date & time = 01-01-06 01:20:50

Measurement Condition

X-ray tube

target = Cu
voltage = 40.0 (kV)
current = 30.0 (mA)

Slits

divergence slit = 1.00000 (deg)
scatter slit = 1.00000 (deg)
receiving slit = 0.30000 (mm)

Scanning

drive axis = Theta-2Theta
scan range = 10.000 -80.000
scan mode = Continuous Scan
scan speed = 6.0000 (deg/min)
sampling pitch = 0.0200 (deg)
preset time = 0.20 (sec)

No.	<2Theta>	<d >	<l >	<l/Io>	<FWHM >	<integrated I>
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2	11.5200	7.67524	3	4	0.0400	20
3	12.3250	7.17568	3	4	0.0500	23
4	13.2500	6.67675	5	7	0.1800	82
5	14.1700	6.24525	7	9	0.2600	144
6	14.9000	5.94088	9	12	0.6400	450
7	15.7600	5.61858	6	8	0.0000	0
8	16.3400	5.42042	14	18	1.0000	1279
9	17.6000	5.03511	20	26	0.0000	0
10	17.7000	5.00688	17	22	0.0000	0
11	18.9400	4.68179	30	39	2.1600	3540
12	20.1600	4.40113	51	67	0.0000	0
13	20.5200	4.32473	57	75	0.0000	0
14	21.2400	4.17972	76	100	0.0000	0
15	22.2600	3.99045	63	83	0.0000	0
16	22.6600	3.92091	57	75	0.0000	0
17	22.9400	3.87368	55	72	0.0000	0
18	23.7200	3.74804	40	53	0.0000	0
19	24.4800	3.63337	21	28	0.8400	1515
20	25.8900	3.43860	12	16	1.6200	905
21	27.7300	3.21447	2	3	0.3000	55
22	28.4500	3.13474	3	4	0.1000	43
23	29.4100	3.03456	3	4	0.1000	33
24	30.8000	2.90071	7	9	0.2000	146
25	31.7900	2.81259	2	3	0.0600	20
26	32.8500	2.72422	4	5	0.1000	46
27	34.6300	2.58816	8	11	0.3800	253
28	36.0300	2.49074	3	4	0.0600	24
29	38.6150	2.32974	4	5	0.1300	50
30	40.6000	2.22030	2	3	0.0400	12
31	43.1500	2.09481	3	4	0.0600	29
32	45.5233	1.99096	4	5	0.0333	22
33	46.9600	1.93334	4	5	0.2400	158
34	48.7950	1.86484	5	7	0.1900	135
35	49.3800	1.84411	2	3	0.0800	34
36	50.5800	1.80314	3	4	0.0400	17
37	52.8500	1.73091	2	3	0.0600	23
38	54.3000	1.68806	2	3	0.0400	12
39	55.3900	1.65740	3	4	0.0600	30
40	56.3300	1.63195	3	4	0.1800	50
41	57.4900	1.60175	2	3	0.6200	64
42	64.1100	1.45139	4	5	0.2200	73
43	64.9200	1.43522	3	4	0.0800	27
44	66.4000	1.40678	3	4	0.2000	46
45	67.2200	1.39160	4	5	0.2400	101

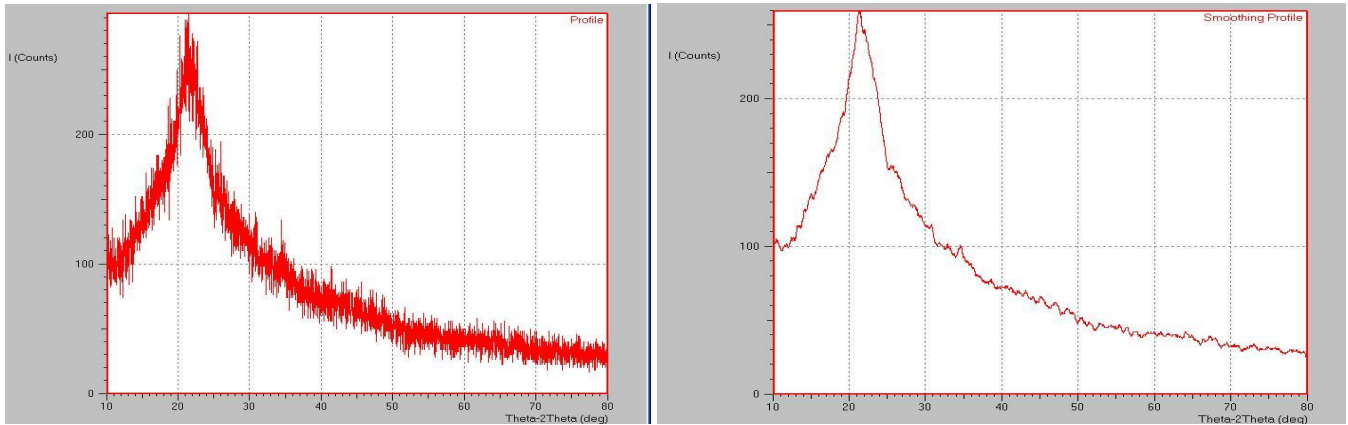


Fig 2: BF-Leaf Powder-male

Data : BF-LeafPowder-Female
 File Name : BF-LeafPowder-Female.PKR

Peak Datafile
 comment = BF-LeafPowder-Female
 date & time = 01-01-06 01:07:15

Measurement Condition

X-ray tube
 target = Cu
 voltage = 40.0 (kV)
 current = 30.0 (mA)

Slits

divergence slit = 1.00000 (deg)
 scatter slit = 1.00000 (deg)
 receiving slit = 0.30000 (mm)

Scanning

drive axis = Theta-2Theta
 scan range = 10.000 -80.000
 scan mode = Continuous Scan
 scan speed = 6.0000 (deg/min)
 sampling pitch = 0.0200(deg)
 preset time = 0.20 (sec)

No.	<2Theta>	<d>	<I>	<I/Io>	<FWHM>	<integrated I>
1	10.4100	8.49101	6	7	0.3400	181
2	11.8900	7.43721	2	2	0.0600	10
3	12.8200	6.89971	2	2	0.1200	25
4	13.4050	6.59989	3	4	0.0500	13
5	14.7500	6.00096	11	13	0.5800	389
6	15.5400	5.69762	11	13	0.4000	288
7	17.1600	5.16321	22	27	1.6800	1864
8	18.1000	4.89713	25	30	0.0000	0
9	18.9800	4.67201	32	39	0.0000	0
10	20.0800	4.41849	50	60	0.0000	0
11	21.0600	4.21504	71	86	0.0000	0
12	21.8200	4.06992	83	100	3.4800	7266
13	23.7200	3.74804	42	51	1.9600	2721
14	24.7200	3.59863	21	25	1.2400	864
15	25.6400	3.47156	10	12	1.0000	412
16	26.4100	3.37206	10	12	0.5400	331
17	27.6600	3.22245	2	2	0.0000	0
18	28.3750	3.14285	2	2	0.0500	6
19	29.3700	3.03860	6	7	0.1400	83
20	31.1450	2.86936	4	5	0.0900	36
21	32.1500	2.78192	2	2	0.0600	7
22	33.5700	2.66742	4	5	0.1000	28
23	34.7150	2.58202	6	7	0.8100	285
24	36.1800	2.48075	4	5	0.1200	40
25	37.0300	2.42574	2	2	0.0600	12
26	37.9750	2.36752	3	4	0.1100	45
27	40.6500	2.21768	4	5	0.1400	71
28	42.6900	2.11631	3	4	0.1400	58
29	43.7800	2.06611	6	7	0.2800	126
30	44.8850	2.01778	6	7	0.4300	150
31	45.9600	1.97306	3	4	0.0400	19
32	46.7800	1.94036	3	4	0.0400	21
33	49.6250	1.83558	3	4	0.0300	19
34	51.2600	1.78080	2	2	0.3200	74
35	56.1200	1.63756	3	4	0.0400	25
36	57.4700	1.60226	2	2	0.1800	35

37	59.6800	1.54809	3	4	0.0400	23
38	62.7000	1.48059	4	5	0.2400	68
39	63.7200	1.45933	3	4	0.1200	48
40	64.4700	1.44415	2	2	0.1400	40
41	65.6800	1.42044	2	2	0.0400	9
42	66.8600	1.39821	2	2	0.0400	10
43	67.7700	1.38164	2	2	0.0600	14
44	69.8600	1.34533	2	2	0.0400	12
45	72.9600	1.29562	4	5	0.2400	88

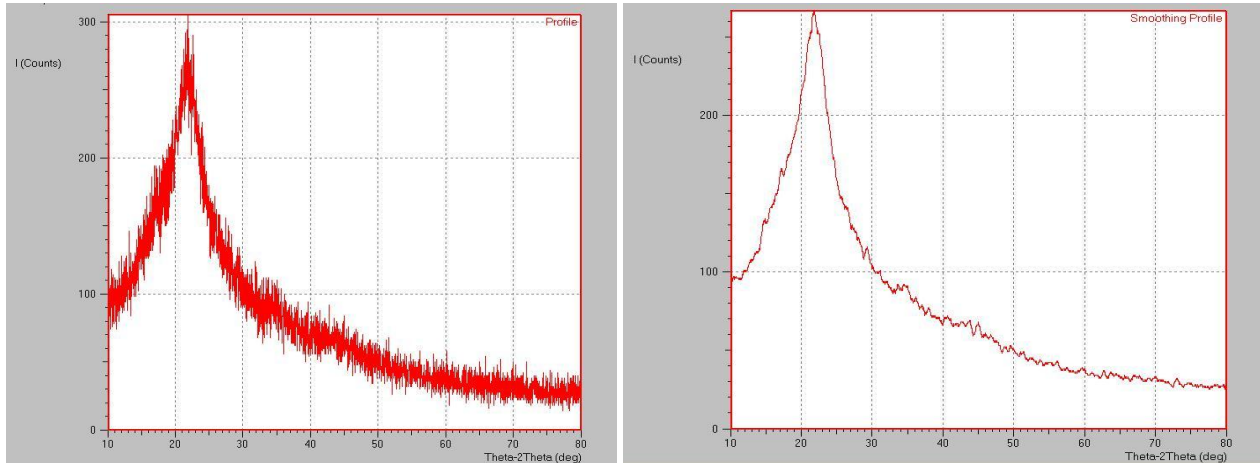


Fig 3: BF-Leaf Powder-Female

4. Conclusion

The Palmyra palm (*Borassus flabellifer*), a multipurpose tree of great utility, occurs extensively in Tamil Nadu state, India. *Borassus flabellifer* Increasing exploitation of the Palmyra threatens the future supply of palm raw materials so important to rural populations. The *Borassus flabellifer* leaves could be considered as good sources of natural antioxidants and antimicrobials and may find several applications in agro-food and pharmaceutical industries. Study of characterizing the *Borassus flabellifer* is going and result will be shown in next publication.

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