International Journal of Physics and Applications

E-ISSN: 2664-7583
P-ISSN: 2664-7575
IJOS 2024; 6(1): 03-07

www.physicsjournal.in
Received: 13-11-2023
Accepted: 14-12-2023

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Structural and spectral analysis of green synthesized zinc oxide nanoparticles

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DOI: https://doi.org/10.33545/26647575.2024.v6.i1a.77

Abstract
Plants are good replacement of hazardous chemicals used as capping agents for synthesizing the nanoparticle. Green synthesis of ZnO nanoparticles is performed using aloe-vera gel as capping agent and obtained nanoparticles are calcined at 400 °C. The XRD pattern of prepared ZnO nanoparticles are obtained and denoised using Haar wavelet transforms. The sharp peaks of XRD pattern indicates crystallite nature of ZnO nanoparticles. Interplanar spacings calculated by using Bragg's equations are compared with standard JCPDS data. The structural properties are very close to standard JCPDS data which confirm that synthesized nanoparticles are pure and crystallite in nature.

Keywords: Denoising, green synthesis, nanoparticles, wavelet transforms, zinc oxide

Introduction
Nanoparticles are very small sized particles (range from 10nm-100nm) with increased chemical activity, thermal conductivity and non-linear optical performance by virtue of their large surface area to volume ratio [1]. Zinc oxide has economical and industrial interest due to wide range of applicability in different areas such as rubber industry, biomedical field and metal surface treatment. Zinc Oxide nanoparticles are being used in various healthy food and cosmetic industry of consumer which calls for environment friendly access to their synthesis [2]. Zinc oxide has attracted great interest of researchers due to its optical, piezoelectric, magnetic and gas sensing properties. With these properties, ZnO nanostructure also has high catalytic efficiency and strong absorption ability. It is frequently used in manufacture of sunscreens [3], ceramic, wastewater treatment and as fungicide [4-5]. Green synthesis of nanoparticles is a method performed by using plant parts extract like leaves, roots and stems etc. Green synthesis approach to form nanoparticles is an ecofriendly, cost effective and safe [6]. Green synthesized ZnO nanoparticles are free from additional impurities. Plant parts such as roots, leaves, seeds, stems, fruits are used for the nanoparticles synthesis because their extract is rich in phytochemicals which acts as reducing and stabilization agent both.

Wavelet transforms is a new and favourable set of tools and techniques widely used to analyse the signals, especially non-stationary and transient signals [7]. A wavelet refers to a zero average oscillating function which is well localized over a short period of time. The family of wavelets is obtained by translating and dilating the original function called mother wavelet. Wavelet transform like Fourier transform is a magical mathematical tool used to analyse many problems in science and engineering. Multiresolution analysis (MRA) is a recursion technique of analysis in which signal is analysed as per required level of decomposition [8]. In signal denoising, the wavelet coefficients below threshold value are eliminated and the inverse wavelet transformed is obtained [9]. The denoised XRD patter of zinc oxide nanoparticles provides signal and peaks with more clarity.

Zinc oxide nanoparticles have tremendous semiconducting properties because of its large band gap (3.37eV) and high exciton binding energy (60meV), high photocatalytic activity, U-V absorption properties and anti-inflame properties. Due to its U-V absorption properties, it has been largely used in cosmetic like sunscreen lotion [10]. They are also being used for manufacturing of rubber and paint, for water remediation, protein absorption and dental related applications [11].

Literature Review

A lot of work has been done to synthesize ZnO nanoparticle using extract of different parts of plants, fungus, algae, bacteria and other. ZnO nanoparticles may also be prepared via physical, chemical, and biological methods. Chemical methods may involve precipitation, microemulsion, chemical reduction, like hydrothermal techniques, which may lead to high energy consumption and need high pressure or temperature conditions in the process [12]. The sol-gel synthesis method is the most commonly used method among the chemical methods. In sol-gel method a zinc precursor salt (nitrate, sulphate, chloride, etc.) and a chemical reagent are used for regulating pH of the solution and avoid the residuals of $Zn(OH)_2$. After this, the solution will be calcined to thermal treatment under temperatures up to 1000 °C to obtain the ZnO nanoparticles [13]. Although ZnO nanoparticles are synthesized via physical techniques by vapor deposition, plasma and ultrasonic irradiation [14]. Nonetheless, these techniques require a high amount of energy and costly equipment, so that cost of the products is increased. Another approach to obtain ZnO nanoparticles is using green synthesis, which has developed as an alternative eco-friendly process.

Discrete wavelet analysis is performed by a fundamentally new iterative method called multiple-resolution analysis (MRA). Mallat and others [15-17] introduced MRA consisting a sequence$V_j : j \in \mathbb{Z}$ of closed subspaces of $L^2(\mathbb{R})$, a Lebesgue space of square integrable functions, satisfies the following properties as follows: -

1. $V_{j+1} \subset V_j : j \in \mathbb{Z}$
2. $\cap_{j\in\mathbb{Z}} V_j = \{0\}$, $\cup_{j\in\mathbb{Z}} W_j = L^2(\mathbb{R})$,
3. For every, $L^2(\mathbb{R})$, $f(x) \in V_j \Rightarrow f(2x) \in V_{j+1}, \forall j \in \mathbb{Z}$
4. For a function $\phi(x) \in V_0$ the function $\{\phi(x-k): k \in \mathbb{Z}\}$ is orthonormal basis of V_0.

Here, the function $\phi(x)$ is called a scaling function of given MRA and property 3) implies a dilation equation as following: -

$$\phi(x) = \sqrt{2}\ \sum_{k\in\mathbb{Z}} \alpha_k\ \phi(2x-k)$$

Where h_k is called low pass filter, defined as follows: -

$$\alpha_k = \int_{-\infty}^{\infty} \phi(x)\phi(2x-k)\, dx$$

The function ψ, that is wavelet function can be expressed as follows: -

$$\psi(x) = \sqrt{2}\ \sum_{k\in\mathbb{Z}} \beta_k\ \phi(2x-k)$$

Where $\beta_k = (-1)^{k+1}\alpha_{1-k}$ are high pass filters. From conditions of multiresolution analysis (MRA) and elementary functional analysis, each space V_j can be expressed as combination of two subspace V_{j+1} and W_{j+1} such that every function f in V_j can be uniquely decomposed into $f = u + v$ with $u \in V_{j+1}$ and $v \in W_{j+1}$. We write this as follows: -

$$V_j = V_{j+1} \oplus W_{j+1},\ \forall j \in \mathbb{Z}$$

If all such functions u and v are orthogonal ($\langle u, v\rangle = 0$), then W_{j+1} is the orthogonal complement of V_{j+1} in V_j ($V_{j+1} \perp W_{j+1}$) and the construction below will give the scaling function and mother wavelet of an orthonormal wavelet basis for $L^2((\mathbb{R})$. By MRA, the orthogonal decomposition of space $L^2(\mathbb{R})$ is as following: -

$$L^2(\mathbb{R}) = \sum_j V_j = \sum_j W_{j+1} \oplus W_{j+2} \oplus W_{j+3} \ldots\ldots \oplus W_{j_0} \oplus V_{j_0}$$

Any discrete signal in square summable space $\ell^2(\mathbb{Z})$ can be expressed as follows: -

$$f[n] = \frac{1}{\sqrt{M}} \sum_k a[j_0, k]\phi_{j_0,k}[n] + \frac{1}{\sqrt{M}} \sum_{p=j+1}^{j_0} \sum_{k\in\mathbb{Z}} d[p,k]\psi_{p,k}[n]$$

Here $f[n]$, $\phi_{j_0,k}[n]$ and $\psi_{p,k}[n]$ are discrete functions having total M points defined in interval $[0, M-1]$. The wavelet coefficients can be derived as follows: -

$$a[j_0, k] = \frac{1}{\sqrt{M}} \sum_n f[n]\ \phi_{j_0,k}[n]$$

$$d[p, k] = \frac{1}{\sqrt{M}} \sum_n f[n]\ \psi_{p,k}[n]$$

with $j < p \leq j_0$, where $a[j_0, k]$ and $d[j, k]$ are known as approximation and detailed coefficients respectively.

Thresholding is a technique performing to zero out arbitrary small magnitude wavelet coefficient (Below threshold) and retain the large magnitude wavelet coefficients (Above threshold) [18]. Threshold operator is operated on wavelet coefficients and it preserves certain coefficients above threshold (τ) and zero out remaining coefficients. Threshold operator may be defined as: -

$$\{T_\lambda\}_{j,k} = \begin{cases} d[j,k], & |d[j,k]| \geq \tau \\ 0, & \text{otherwise} \end{cases}$$

The quantized wavelet coefficients are used to reconstruct a version of input via an appropriate reconstruction algorithm.

Materials and Methods

The green synthesis approach of ZnO nanoparticles is performed in the following steps: -

Materials and Extraction of Plant

The zinc nitrate hexahydrate was purchased from M.S. Scientific. Fresh leaves of aloe-vera are collected from 187/6B, Buddhi Vihar, Moradabad. Leaves were washed under running tape water for 5-10 minutes and dried for 30 minutes. Gel of aloe-vera leaves was extracted using stained steels knife and filtered for removing impurity. Gel was stirred vigorously at room temperature for getting homogeneous gel and stored in refrigerator for further use (Fig.1).

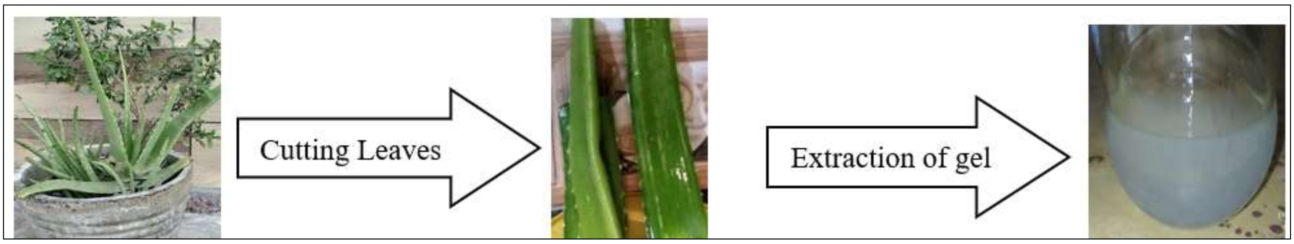

Fig 1: Extraction of Aloe-Vera Gel

Method

The current research work was done at Department of Physics, Hindu College Moradabad. A solution of 0.1 molarity is prepared using distilled water and zinc nitrate hexahydrate ($Zn(NO_3)_2 \,.6H_2O$). Aloe-vera gel (25 ml) is added slowly to prepare solution (200 ml) under vigorous stirring at room temperature. The colour of solution was milky green. The solution was stirred continuously at 75 °C temperature until colour of solution changed and gel like solution obtained. The changing in colour of the solution was indication of complete reaction and it was visual confirmation of nanoparticles. The prepared nanoparticles in gel form were calcined at 400 °C in hot air oven for 1 hour. The sample was crushed for 15 minute using mortar and pestle for getting fine powdered form of prepared nanoparticles (Fig. 2).

Fig 2: Green Synthesis of Zinc Oxide Nanoparticles

The XRD pattern of as prepared sample is obtained and denoised by wavelet transforms. The signal denoising is implemented by software dyadWaves. With help of denoised XRD pattern, structural properties of the green synthesized ZnO nanoparticles are determined and discussed.

Results and Discussions

The XRD pattern of as prepared ZnO nanoparticles using X-ray wavelength 1.540 Angstrom, is shown in Fig. 3.

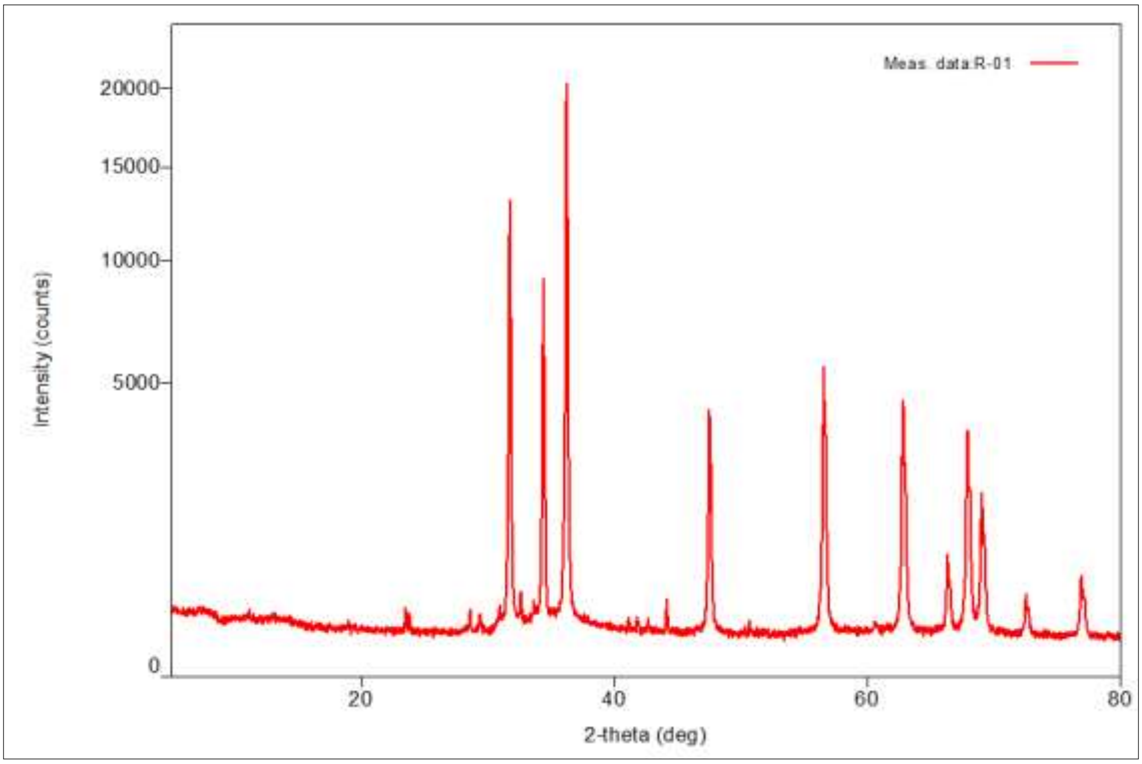

Fig 3: XRD Pattern of ZnO Nanoparticles

The sharpness of peaks indicates that the obtained sample is crystallite in form. The denoised XRD is obtained using Haar wavelet transforms, level-1 (Fig. 4).

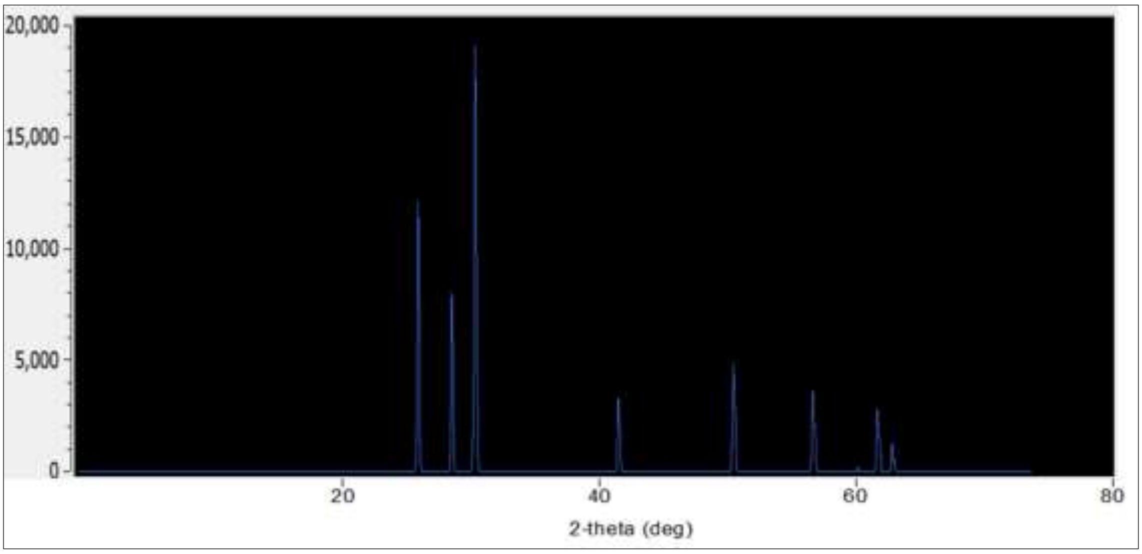

Fig 4: denoised XRD Pattern

Interplanar spacings are calculated by using Bragg's equation, $2dsin\theta = n\lambda$, where n is the order of diffraction, λ is the wavelength of X-ray and d is interplanar spacing between given plane $(h\ k\ l)$. The interplanar d-spacings ($d_{h\ k\ l}$) and full width at half maxima (FWHM) values obtained from XRD synthesized ZnO are shown in table 1.

Table 1: Calculation of interplanar spacings and comparison with standard JCPDS data

Peak (2θ)	θ	$sin\theta$	$d = n\lambda/2sin\theta$ (Å)	d (JCPDS) Å	d(nm)	(h k l)	FWHM (Degree)
31.740	15.8700	0.2735	2.8154	2.8135	0.28154	1 0 0	0.125
34.391	17.1995	0.2957	2.6040	2.6027	0.26040	0 0 2	0.119
36.222	18.1110	0.3109	2.4767	2.4751	0.24767	1 0 1	0.133
47.507	23.7535	0.4028	1.9116	1.9106	0.19116	1 0 2	0.134
56.555	28.2773	0.4737	1.6255	1.6244	0.16255	1 1 0	0.147
62.823	31.4115	0.5212	1.4774	1.4769	0.14774	1 0 3	0.159
66.336	33.1680	0.5471	1.4074	1.4070	0.14074	2 0 0	0.168
67.914	33.9570	0.5586	1.3784	1.3780	0.13784	1 1 2	0.175
69.047	34.5235	0.5667	1.3587	1.3580	0.13587	2 0 1	0.170

The diffraction peaks corresponding to planes (100), (002), (101), (102), (110), (103), (200), (112) and (201) obtained from XRD data are compatible with JCPDS (Card No. 01-089-0510) which indicates hexagonal wurtzite phase of ZnO nanoparticles. In ZnO wurtzite structure oxygen atoms are joined with zinc atoms such that they form a hexagonal closed pack type structure. The structural properties of green synthesized zinc oxide nanoparticles show strong agreement with the standard JCPDS data.

Conclusion

Green route to obtain ZnO nanoparticle is an eco-friendly, cost effective and simple approach. ZnO nanoparticles are synthesized using aloe-vera gel as a capping agent. The XRD pattern is obtained for knowing the structural properties. The sharp peaks confirm the crystal nature of the sample. The XRD pattern is denoised using Haar wavelet transforms, level-1. The interplanar d-spacings $d_{h\ k\ l}$) and full width at half maxima (FWHM) values are determined. The structural properties of ZnO nanoparticles show strong agreement with the standard JCPDS data. The structural study of prepared ZnO nanoparticles confirm its purity and crystallite in nature.

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