World Journal of
Pharmacy and Medical Science

ISSN: 3049-3501
Impact Factor: 5.157
CODEN (USA): WJPMAA

Review Article
2026 Volume 2, Issue 8
Page No.: 144-152

APPLICATION OF X-RAY DIFFRACTION (XRD) IN THE CHARACTERIZATION AND STANDARDIZATION OF AYURVEDIC BHASMAS AND HERBO-MINERAL FORMULATIONS: A COMPREHENSIVE REVIEW

Dr. Anil Kumar*[1], Dr. Manisha Goyal[2], Prof. (Dr.) Govind Sahay Shukla[3], Prof.(Dr.) Rajaram Agarwal[4], Dr. Sangeeta Indoria[5], Dr. Ravi Pratap Singh[6]

[1]MD Scholar, PG Department of Rasa Shastra evam Bhaishajya Kalpana, Post Graduate Institute of Ayurveda, DSRRAU, jodhpur, Rajasthan, india.
[2]Associate Professor, PG Department of Rasa Shastra evam Bhaishajya Kalpana, DSRRAU, Jodhpur, Rajasthan, India.
[3]Vice Chancellor, DSRRAU, Jodhpur, Rajasthan, India.
[4]Professor and HOD, PG Department of Rasa Shastra evam Bhaishajya Kalpana, Post Graduate Institute of Ayurveda, DSRRAU, Jodhpur, Rajasthan, India.
[5,6]Assistant Professor, PG Department of Rasa Shastra evam Bhaishajya Kalpana, Post Graduate Institute of Ayurveda, DSRRAU, Jodhpur, Rajasthan, India.

Article Received: 22 June 2026 Article Review: 13 July 2026 Article Accepted: 03 July 2026

***Corresponding Author: Dr. Anil Kumar**
MD Scholar, PG Department of Rasa Shastra Evam Bhaishajya Kalpana,Post Graduate institute of Ayurveda,DSRRAU , Jodhpur, Rajasthan, India.
DOI: https://doi.org/10.5281/zenodo.21991901

How to cite this Article: Dr. Anil Kumar, Dr. Manisha Goyal, Prof. (Dr.) Govind Sahay Shukla, Prof.(Dr.) Rajaram Agarwal, Dr.Sangeeta Indoria, Dr. Ravi Pratap Singh (2026). APPLICATION OF X-RAY DIFFRACTION (XRD) IN THE CHARACTERIZATION AND STANDARDIZATION OF AYURVEDIC BHASMAS AND HERBO-MINERAL FORMULATIONS: A COMPREHENSIVE REVIEW. World Journal of Pharmacy and Medical Science, 2(8): 144-152.

ABSTRACT

Ayurvedic herbo-mineral formulations, particularly Bhasmas and Rasa preparations, undergo complex pharmaceutical processing procedures such as Śodhana and Māraṇa to convert raw metals and minerals into therapeutically safe and bioavailable forms. Modern analytical techniques are essential for validating these traditional preparations and ensuring their quality, safety, and standardization. X-ray diffraction (XRD) is a non-destructive analytical technique widely used for phase identification, crystallinity assessment, and structural characterization of crystalline materials. The present review focuses on the application of XRD in the characterization of various Ayurvedic single-drug Bhasmas and herbo-mineral formulations, including Lauha Bhasma, Yashada Bhasma, Tamra Bhasma, Swarna Bhasma, Makaradhwaja, Vasantakusumakar Rasa, Trivanga Bhasma, and Tarakeswara Rasa. XRD studies revealed the disappearance of elemental metal peaks and the appearance of stable oxide and sulfide phases such as Fe_2O_3, ZnO, SnO_2, CuO, and HgS, confirming successful detoxification and phase transformation during pharmaceutical processing. Peak broadening and variation in diffraction intensity indicated reduction in crystallite size and formation of nano- or microcrystalline structures, which may contribute to enhanced bioavailability and therapeutic efficacy. The review highlights the importance of XRD as a scientific tool for confirming phase purity, structural stability, reproducibility, and standardization of Ayurvedic formulations. The integration of traditional Ayurvedic knowledge with modern analytical characterization techniques can significantly improve quality control and support the global acceptance of Ayurvedic herbo-mineral medicines.

KEYWORDS: X-ray diffraction, Herbo-mineral formulations, Bhasma, Quality control.

INTRODUCTION

In recent years, the use of herbo-mineral medicines has increased greatly. With this rise in use, concerns about the quality of these medicines have also grown. For these medicines to be useful and trustworthy, they must be safe to consume, effective in treatment, and free from harmful or toxic effects.[1]

In Ayurveda, Bhasmas prepared from the seven metals constitute some of the most important medicines. During their stepwise preparation, the raw metals are processed with specific herbal materials, which helps in detoxification, conversion into a form that is easily absorbed by the body, and enhancement of therapeutic potency and efficacy. Properly prepared Bhasmas are believed to eliminate the root cause of disease and strengthen the body's natural defense mechanisms. However, literature reviews indicate that many Bhasmas currently available in the market do not fully achieve these intended effects. Therefore, the use of modern screening and analytical techniques such as XRD and EDAX is essential for the standardization and wider acceptance of Bhasmas at both national and international levels.[2]

Recent developments in analytical techniques such as X-ray diffraction (XRD), field emission scanning electron microscopy, and energy-dispersive X-ray analysis have made it possible to study the structure and properties of drugs at the atomic and molecular levels. In the Ayurvedic pharmaceutical industry, these techniques are used to analyze raw materials and finished products, helping in their proper characterization and in validating this ancient system of medicine using modern scientific standards.[3]

MATERIALS AND METHODS

The present review was conducted using published scientific literature related to XRD analysis of Ayurvedic Bhasmas and herbo-mineral formulations. Relevant research articles and analytical studies were collected from peer-reviewed journals and scientific databases. Data regarding diffraction peaks, crystalline phases, phase transformation, and crystallite size were compiled and comparatively analyzed. The XRD findings were interpreted based on standard crystallographic principles to evaluate structural changes, detoxification, and standardization of Ayurvedic formulations.

Principle of X-Ray Diffraction

X-ray diffraction (XRD) is a non-destructive analytical technique based on the elastic scattering of monochromatic X-rays by the periodic atomic planes of crystalline materials. When incident X-rays interact with the electron clouds of atoms in a crystal lattice, scattered waves undergo constructive interference only at specific angles, producing characteristic diffraction peaks. This phenomenon is governed by Bragg's law ($n\lambda = 2d\ sin\theta$), which relates the wavelength of X-rays, interplanar spacing, and diffraction angle. Each crystalline phase generates a unique diffraction pattern, allowing phase identification and structural characterization through analysis of peak positions, intensities, and widths.[4]

Components of an X-Ray Diffraction (XRD) Instrument[4]

An X-ray diffraction (XRD) instrument consists of several key components that function collectively to generate, detect, and analyze diffraction patterns for material characterization.

1. **X-ray Source**

The X-ray source generates monochromatic X-rays, typically using Cu-Kα or Mo-Kα radiation, which are directed toward the sample for diffraction analysis.

2. **Goniometer**

The goniometer provides precise angular positioning and controlled rotation of both the sample and detector, enabling accurate measurement of diffraction angles (2θ).

3. **Sample Stage (Sample Holder)**

The sample stage securely holds the specimen in the path of the incident X-ray beam and ensures proper alignment during data acquisition.

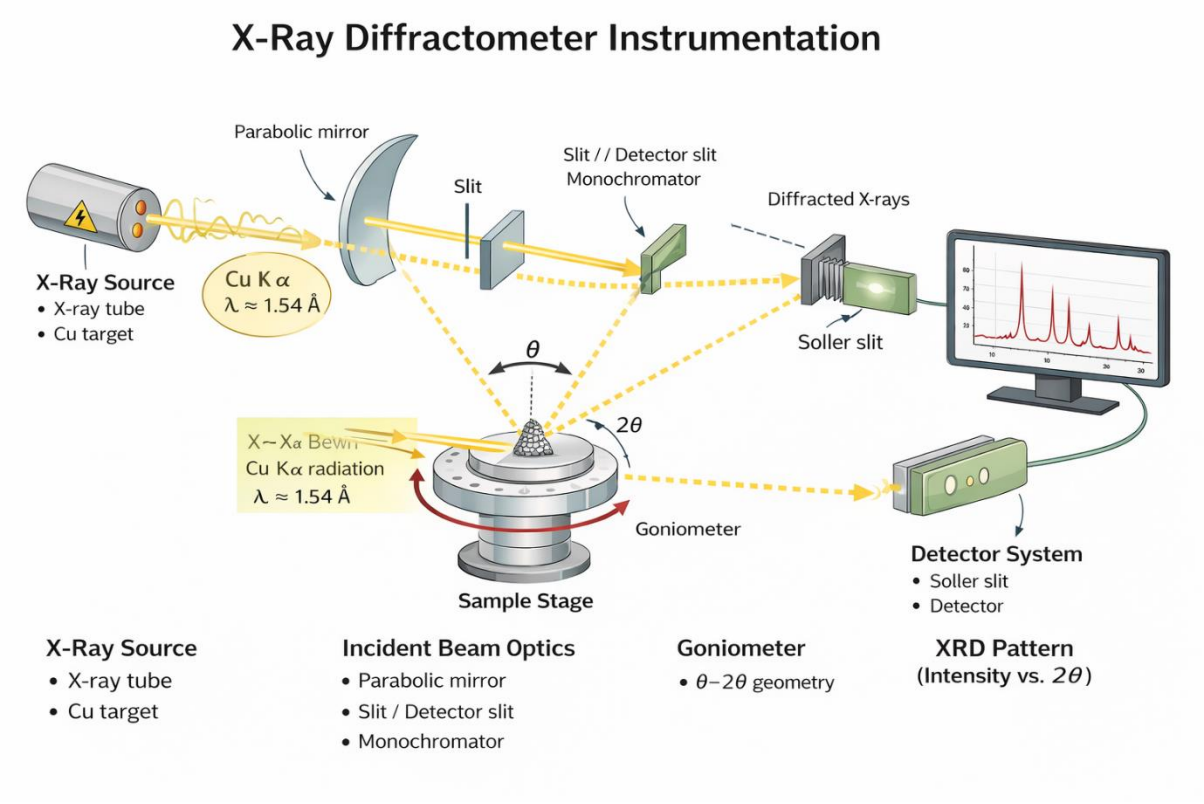
4. **Detector**

The detector captures the diffracted X-rays emerging from the sample and converts the detected radiation into electrical signals proportional to the diffraction intensity.

5. **Data Acquisition and Processing System**

The acquired diffraction data are processed using specialized software to generate diffraction patterns, which are subsequently analyzed to determine crystal structure, phase composition, crystallinity, lattice parameters, and other structural characteristics of the material.

Together, these components enable the accurate characterization of crystalline materials through the measurement and interpretation of X-ray diffraction patterns.



Applications of X-Ray Diffraction (XRD)[5]

X-ray diffraction (XRD) is a versatile and non-destructive analytical technique extensively used for the characterization of crystalline materials. It provides valuable information regarding phase composition, crystal structure, lattice parameters, crystallinity, and microstructural characteristics. XRD is widely employed for phase identification and quantification, as each crystalline material produces a unique diffraction pattern that serves as its structural fingerprint.

The technique also enables determination of crystal symmetry, unit-cell dimensions, and atomic arrangement within a crystal lattice through analysis of diffraction peak positions and intensities.

Furthermore, XRD is commonly utilized to evaluate crystallite size and degree of crystallinity. Crystallite size can be estimated from diffraction peak broadening using the Scherrer equation:

$D = K\lambda / \beta\cos\theta$

where D is the crystallite size, K is the shape factor (generally 0.9), λ is the wavelength of the X-ray radiation, β is the full width at half maximum (FWHM) of the diffraction peak, and θ is the Bragg diffraction angle.

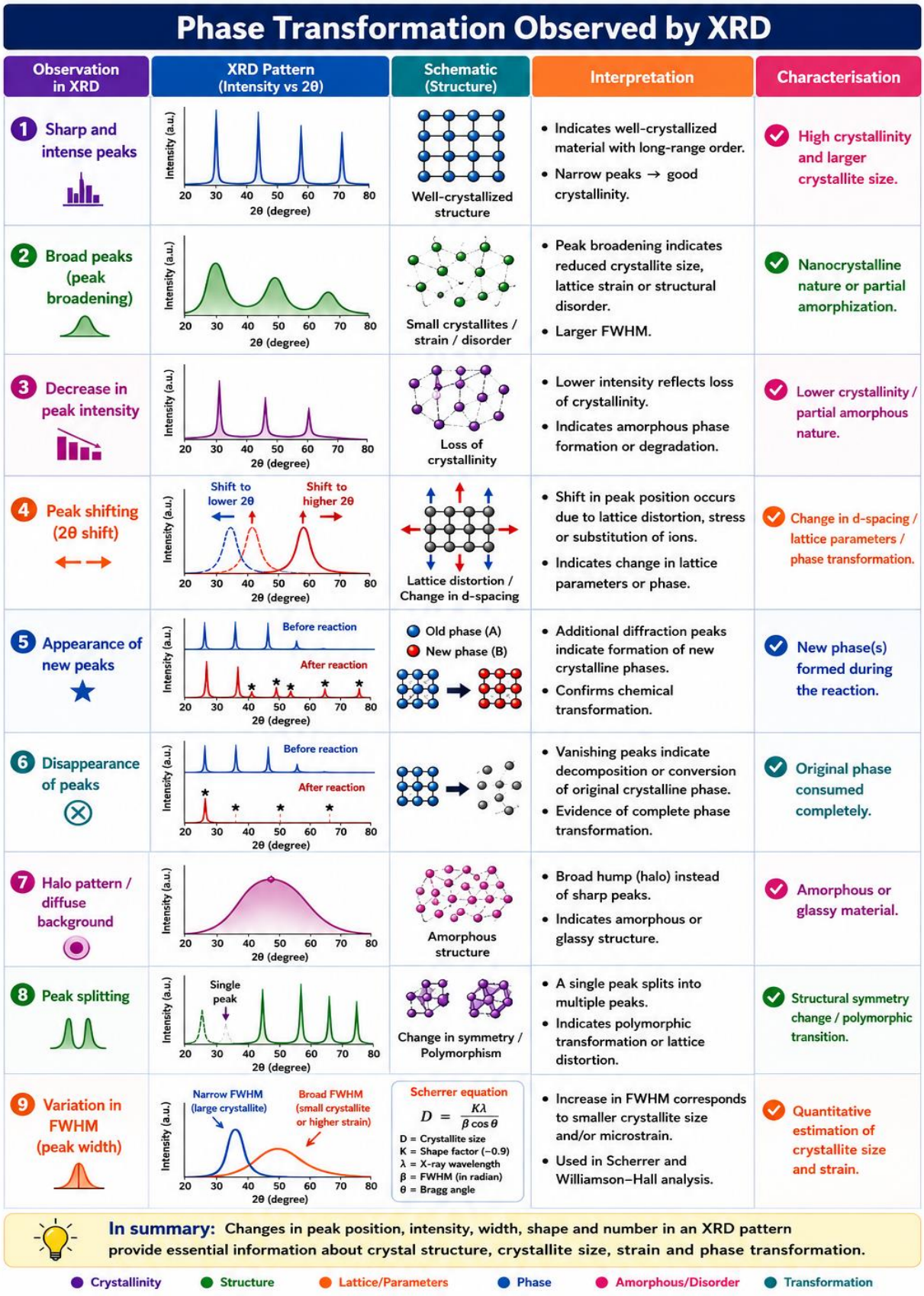
In addition, XRD is an effective tool for investigating phase transformations, residual stress and strain, dislocation density, crystallographic orientation (texture), and thermal expansion behavior of materials. Owing to its ability to provide detailed structural and compositional information without damaging the sample, XRD has become an indispensable technique in mineralogy, materials science, metallurgy, nanotechnology, and pharmaceutical research.

Advantages of X-Ray Diffraction (XRD)

- Non-destructive technique for the characterization of crystalline materials.
- Enables identification and quantification of crystalline phases.
- Provides information on crystal structure, lattice parameters, and crystallographic orientation.
- Useful for determining crystallite size, crystallinity, and phase transformations.
- Facilitates the evaluation of residual stress, strain, and crystal defects.

Limitations of X-Ray Diffraction (XRD)

- Primarily applicable to crystalline materials and has limited sensitivity toward amorphous phases.
- Peak overlap in complex multiphase systems can complicate phase identification.
- Requires careful sample preparation and powdered, homogeneous specimens.
- Quantitative results may be influenced by preferred orientation, particle size effects, and instrumental errors.
- Detection of minor phases is limited, and data interpretation often requires specialized expertise.



XRD Analysis of Ayurvedic Single-Drug Bhasma

Hīrak Bhasma:[6]

XRD revealed peaks of hematite (Fe_2O_3) and quartz (SiO_2), with absence of diamond carbon peaks, confirming complete structural transformation during Māraṇa. Peak broadening indicated micro- to nano-crystalline nature favorable for therapeutic assimilation.

Maṇḍūra Bhasma:[7] XRD showed predominant hematite (Fe_2O_3) phases with no elemental iron, confirming effective oxidation and detoxification. Stable peak positions supported chemical stability of the prepared Bhasma.

Abhraka (Mica) Bhasma:[8]
Characteristic peaks of $KMg_3(Si_3Al)O_{10}(OH)_2$ confirmed retention of silicate framework with modified crystallinity. Peak broadening indicated nanocrystalline domains without destruction of mineral structure.

Rājata (Silver) Bhasma[2]
XRD patterns showed silver oxide and crystalline silver phases with reduced peak intensity, indicating fine particle size and partial amorphization. Absence of metallic silver confirmed complete Bhasmīkaraṇa.

Vaṅga (Tin) Bhasma:[9]
Progressive transformation from metallic tin to tin dioxide (SnO_2) was observed. Dominant SnO_2 peaks confirmed formation of a stable and pharmacologically safer oxide form.

Tāmra (Copper) Bhasma:[10]
XRD indicated CuO and Cu_2O phases with crystallite size below 100 nm. Absence of metallic copper confirmed thorough oxidation and nanocrystalline nature.

Lauha (Iron) Bhasma:[11]
XRD analysis showed gradual conversion of Fe_3O_4 (magnetite) into stable α-Fe_2O_3 (hematite) during repeated puta at high temperature. The increase in sharp crystalline peaks confirmed oxidation, enhanced crystallinity and successful transformation of raw iron into therapeutically suitable Lauha Bhasma.

Yaśada (Zinc) Bhasma:[12]
Sharp peaks corresponding to hexagonal ZnO confirmed complete conversion of zinc metal into oxide form. Reduced crystallite size supported enhanced stability and bioacceptability.

Swarṇa (Gold) Bhasma:[13]
XRD exhibited characteristic FCC gold reflections (111, 200, 220, 311), confirming crystalline purity. Moderate peak broadening suggested micro- to sub-micron particle size.

Bhasma (Single Drug)	Major 2θ Values (°)	Identified Crystalline Phases	Interpretation / Significance
Hīrak Bhasma[6]	~26.6, 33.2, 35.6	Quartz (SiO_2), Hematite (Fe_2O_3)	Absence of diamond carbon peaks confirms complete structural transformation during Māraṇa
Maṇḍūra Bhasma[7]	~35.50,35.60 48.30	Hematite (Fe_2O_3)	Conversion of raw Mandura into stable iron oxide; no free iron detected
Abhraka Bhasma[8]	8.89°, 26.62°, 28.39°, 35.72°, 45.08°, 54.88°	$KMg_3(Si_3Al)O_{10}(OH)_2$ (Biotite-mica phase)	Retention of silicate framework with nanocrystalline modification
Rājata Bhasma[2]	38.09°, 44.15°, 64.50°, 77.45°	Ag_2O / Silver-based crystalline phases	Reduced particle size and partial amorphization enhance bioavailability
Vaṅga Bhasma[9]	26.61, 33.90, 51.80	Tin dioxide (SnO_2)	Confirms complete oxidation of tin metal after Jāraṇa–Māraṇa
Tāmra Bhasma[10]	32.84°, 46.69°, 49.11° ,28.39°, 31.84°, 35.64°	CuO, Cu_4O_3	Nanocrystalline copper oxides indicate detoxified and bioacceptable form
Lauha Bhasma[11]	~30.0, 35.6, 43.0, 57.2	Magnetite (Fe_3O_4), α-Fe_2O_3	Iron present predominantly as magnetite nano-aggregates; no metallic Fe
Yaśada Bhasma[12]	31.42°, 34.09°, 35.91°, 47.22°	Hexagonal ZnO	Complete transformation of zinc metal into stable oxide phase
Swarṇa Bhasma[13]	37.1, 44.3, 64.5, 77.5	FCC Gold (111), (200), (220), (311)	High-purity crystalline gold with micro-to-submicron particle size

XRD-Observed Structural Changes	Interpretation of XRD Findings	Representative BHASMA formulation
Disappearance of metal (elemental) peaks[12]	Metallic reflections (e.g., Zn, Sn, Fe^0, Cu^0) present in raw metal vanish after processing — indicates oxidation/chemical conversion.	Zn metal peaks → ZnO (hexagonal) in Yaśada. Raw Zn peaks gone in bhasma.
Appearance of metal-oxide / compound phases[9]	New peaks correspond to oxides/compounds SnO_2,$K_2Sn_2O_3$ showing chemical transformation.	RaW Sn / Sn + intermediates → dominant SnO_2 in Vaṅga Bhasma.
Phase transition / oxidation state change[11]	XRD shows e.g. Fe_3O_4 ↔ Fe_2O_3 transitions; heating drives Fe(II) → Fe(III), producing the	Raw magnetite or iron turnings → α-Fe_2O_3 in Lauha/Mandur Bhasma

	more stable oxide (α-Fe_2O_3) in final product.	
Peak broadening (increased FWHM)[8]	Broader diffraction peaks → smaller crystallite size / nanocrystalline domains (Debye–Scherrer).	Abhraka: peaks broaden progressively after shodhana/dhanyabhraka/marana → crystallite size ↓.
Shift in relative peak intensities / new peak positions[12]	Incorporation of herb-derived elements or formation of mixed phases gives changes in intensities and new d-spacings.	Yashada: raw shows Zn metal peaks; bhasma shows distinct ZnO peak set (new 2θ positions/intensities).
Reduction of crystalline purity / partial amorphization[2]	Processed samples sometimes show weaker or broader peaks (lower crystallinity) indicating formation of amorphous or poorly crystalline organo-metallic composites.	Rājata: reduced intensity / partial amorphization (fine particle size) vs. sharp metal peaks in raw.
Emergence of herb-derived or accessory phases[7]	Peaks from K, Si, Ca, etc., (from herbal media) may appear or increase — shows incorporation of elements from processing media.	Mandur: K, Ca, Si content increases after processing; XRD/EDAX show added phases/traces.
Decrease in coherent domain (crystallite) size (quantified)[12]	Scherrer/peak-width calculations give crystallite-size (nm); processed bhasmas typically show dramatic size reduction (μm → nm).	Yaśada: crystallite size ≈ 32.8 nm (bhasma) vs. ~2000 nm raw (DLS/PSD evidence).
Conversion of complex raw minerals to simpler medicinal phases[6]	Raw complex mineral peaks replaced by simpler, pharmacologically acceptable oxides/crystalline forms used therapeutically.	Hīrak: raw carbon allotrope (diamond) → XRD shows hematite/quartz and other mineral phases in processed bhasma.
Qualitative confirmation of completeness of bhasmīkaraṇa[9]	Presence/absence of original metal peaks or residual phases i+-s used as a QC criterion — XRD confirms "complete" or "incomplete" conversion.	Vanga: Jarita still shows some Sn; after Marana Sn peaks disappear → declared properly processed.

XRD Analysis of Ayurvedic herbo-mineral drugs

X-ray diffraction (XRD) analysis of **Makaradhwaja[14]** revealed characteristic peaks of **mercuric sulfide (HgS)**, confirming complete transformation of mercury and sulfur into a stable cinnabar phase with no free metallic mercury present. Nanoparticle size (~34.96 nm) suggests enhanced bioavailability and therapeutic potential.

The XRD pattern of **Mahalaxmi Vilas Ras**[15] revealed the proper formation of stable crystalline mineral phases in the formulation. Similar XRD patterns in all batches indicated good reproducibility and standardization of the drug.

Powder X-ray diffraction (XRD) analysis of **Vasantakusumākara Rasa[16]** revealed the presence of characteristic crystalline phases corresponding to major mineral constituents of the formulation.The XRD profile confirmed the incorporation of Rasa Sindura, Vanga Bhasma, Naga Bhasma, and Loha Bhasma in stable crystalline form. Similar diffraction patterns obtained in all batches indicated good reproducibility, phase stability, and proper standardization of the herbo-mineral formulation.

Powder X-ray diffraction (XRD) analysis of **Trivanga Bhasma[17]** demonstrated distinct diffraction peaks indicating the presence of crystalline metallic oxide phases of **lead, zinc, and tin**. The intense and sharp diffraction peaks confirmed the highly crystalline nature of the formulation. Comparative XRD profiles of formulated and marketed samples exhibited similar reflection patterns, indicating phase uniformity and reproducibility. Crystallite size calculated using the Scherrer equation was found to be in the nanometer range (~52.7 nm), confirming the nanosized nature of the Bhasma produced after repeated calcination processes.

XRD analysis of **Rasaparpati[18]** showed major diffraction peaks corresponding mainly to metacinnabar (HgS) and free sulfur phases. The study confirmed proper formation of Kajjali and absence of free mercury, indicating successful processing and stability of the formulation.

XRD analysis of **Hridayarnava Rasa[19]** revealed characteristic diffraction peaks corresponding to crystalline phases of copper sulfide (CuS), mercury sulfide (HgS), elemental sulfur, and Cu_2O. The sharp diffraction peaks confirmed the crystalline nature of the formulation and indicated successful conversion of metallic constituents into stable sulfide forms during pharmaceutical processing.

Comparative XRD studies of **Swarna Makṣika Bhasma**[3] demonstrated transformation of raw sulfide ore into **iron-oxide-dominant phases**, highlighting method-dependent phase changes during śodhana and māraṇa Powder X-ray diffraction (XRD) analysis of **Tarakeswara Rasa[1]** demonstrated characteristic crystalline peaks corresponding predominantly to tin-rich astrophyllite and cassiterite (SnO_2) phases. Additional reflections of HgS, HgO, Fe_2O_3, and SiO_2 were also identified. The well-defined diffraction pattern indicated proper pharmaceutical processing and crystallinity of the herbo-mineral formulation.

Formulation	Major XRD Peaks (2θ)	Identified Phases	Inference
Makardhwaja (shadguna balijarita Makardhwaja)[14]	25.0°, 26.7°, 31.4°, 43.8°, 46.0°, 51.9°, 54.8°	Shadguna Kajjali, Mercury sulfide (HgS), Hexagonal, Orthorhombic, Monoclinic phases	Confirms HgS (cinnabar/metacinnabar) as the major crystalline phase, indicating a stable mercurial sulfide form and nanosized particles (~35 nm).
Mahalaxmi Vilas Ras[15]	23.1°, 26.6°, 31.3°, 37.8°, 43.8°, 51.7°	Sulfur, Cinnabar (HgS), Cassiterite (SnO_2), Orpiment (As_2S_3), Zeolite/Mica phases	Confirms the presence of Kajjali, Vanga Bhasma, Haritala, and Abhraka Bhasma, indicating stable crystalline therapeutic phases and proper formulation preparation.
Vasantakusumakar Ras[16]	26.6°, 31.3°, 35.5°, 38.2°, 43.7°, 51.8°	Cinnabar (HgS), Cassiterite (SnO_2), Massicot (PbO), Magnetite (Fe_3O_4), Gold (Au), MgO	Confirms the presence of cinnabar, cassiterite, lead oxide, and iron oxide phases in a stable medicinal form, indicating proper herbo-mineral formulation preparation.
Trivanga Bhasma[17]	34.8°, 36.4°, 49.7°, 55.3°, 63.9°, 65.1°	Lead oxide, Zinc oxide, Tin oxide, crystalline phases	Confirms the crystalline and nanosized nature of Trivanga Bhasma with stable metallic oxide phases formed after calcination.
Rasaparpati[18]	26.3°, 30.5°, 43.7°, 51.8°, 54.2°, 63.6°, 70.0°, 72.2°	Metacinnabar (HgS), Free sulfur	Indicates proper Kajjali formation with stable HgS crystalline phase and absence of free mercury.
Hridayarnava Rasa[19]	23.0°, 26.3°, 27.8°, 33.3°, 35.2°, 43.6°, 51.7°, 54.9°	Copper sulfide (CuS), Mercury sulfide (HgS), Cu_2O	Confirms crystalline sulfide phases of copper and mercury with stable herbo-mineral composition after processing.
Swarna Makshika Bhasma[3]	31.4°, 35.8°, 43.6°, 57.7°, 62.6°	Fe_3O_4, Fe_2O_3, Cu_2O, CuS, $FeSO_4$	XRD analysis confirmed the conversion of raw copper pyrite into stable iron and copper oxide/sulfide phases after Shodhana and Marana, indicating successful Bhasma formation and crystallinity.
Tarakeswara Rasa[1]	26.6°, 31.8°, 33.9°, 51.8°, 65.0°	Tin-rich Astrophyllite, SnO_2, HgS, HgO, Fe_2O_3, SiO_2	XRD study revealed crystalline tin-rich astrophyllite and cassiterite phases, confirming stable multimineral composition and proper herbo-mineral formulation processing.

Phase Transformation Observed by XRD

XRD-Observed Structural Changes	Interpretation of XRD Findings	Representative Herbo-Mineral Formulation
Appearance of new crystalline peaks[3]	Indicates formation of new stable compounds after Shodhana/Marana	Swarna Makshika → Fe_3O_4, Cu_2O, Cu_2S phases in Swarna Makshika Bhasma
Disappearance of original peaks[3]	Shows conversion/removal of raw metallic or mineral phase	Raw $CuFeS_2$ peaks reduced after processing in Swarna Makshika Bhasma
Formation of sulfide phases	Indicates detoxification and stabilization of metals with sulfur	Hg → HgS formation in Rasaparpati[18], Makaradhwaj[14], Mahalaxmi Vilas Ras[15]
Formation of oxide phases	Suggests oxidation during repeated heating/calcination	Fe_2O_3 and SnO_2 formation in Trivanga Bhasma[17] and Tarakeswara Rasa[1]
Sharp and intense peaks[16]	Confirms crystalline and stable structure	Stable HgS crystalline peaks in Vasantakusumakar Ras
Broad peaks/reduced intensity[17]	Indicates reduced crystallite size or nano/micro particles	Trivanga Bhasma showing nanosized crystalline particles
Similar peak pattern in batches[15]	Demonstrates reproducibility and standardization	Similar XRD patterns in Mahalaxmi Vilas Ras batches
Absence of free metal peaks[18]	Confirms proper processing and detoxification	No free mercury peaks detected in Rasaparpati
Presence of multiple mineral phases[1]	Indicates successful incorporation of all ingredients	Tarakeswara Rasa showing SnO_2, HgS, Fe_2O_3, SiO_2 phases
Peak shift/change in intensity[3]	Suggests chemical interaction and phase transformation	Kupipakwa processed Swarna Makshika showing altered crystalline phases

CONCLUSION

The present review highlights the significant role of X-ray diffraction (XRD) as a reliable and non-destructive analytical tool for the characterization and standardization of Ayurvedic herbo-mineral formulations, particularly Bhasmas and Rasa preparations. XRD studies clearly demonstrate that traditional processes such as Śodhana and Māraṇa lead to profound physicochemical transformations, including the conversion of toxic metallic forms into stable, non-toxic oxides or sulfides.

The disappearance of elemental metal peaks and the appearance of well-defined crystalline phases like Fe_2O_3, ZnO, SnO_2, CuO, and HgS confirm successful detoxification and transformation. Additionally, peak broadening and reduced crystallite size observed in many Bhasmas indicate the formation of nano- or micro-crystalline structures, which may enhance bioavailability and therapeutic efficacy.

Furthermore, XRD analysis provides strong scientific validation for classical Ayurvedic concepts, supporting the safety, stability, and effectiveness of properly prepared herbo-mineral medicines. The integration of modern analytical techniques with traditional knowledge is therefore essential for ensuring quality control, reproducibility, and global acceptance of Ayurvedic formulations.

Interpretation

The findings from various XRD studies collectively indicate that Ayurvedic pharmaceutical processes are not merely mechanical but involve complex chemical and structural transformations. These transformations result in:

- **Detoxification:** Toxic metals such as mercury, lead, and copper are converted into stable sulfide or oxide forms (e.g., HgS, PbO, CuO), reducing their toxicity.
- **Phase Transformation:** Raw metallic or mineral phases are transformed into pharmacologically active crystalline compounds.
- **Particle Size Reduction:** Peak broadening in XRD patterns suggests nanocrystalline formation, which may improve absorption and bioavailability.
- **Structural Stabilization:** Formation of thermodynamically stable phases ensures long-term stability and safety of formulations.
- **Incorporation of Herbal Components:** Changes in peak intensities and new phases suggest interaction with herbal media, supporting the concept of organo-mineral complexes.

These interpretations reinforce that properly prepared Bhasmas and Rasa medicines undergo scientifically measurable transformations that align with modern material science principles. Thus, XRD serves as a crucial bridge between traditional Ayurvedic wisdom and contemporary scientific validation, enabling standardization and enhancing credibility at a global level.

Future Scope

Future research should focus on integrating advanced analytical techniques such as XRD with SEM, TEM, ICP-MS, and spectroscopic methods for comprehensive characterization of Bhasmas. Standardization protocols and validated quality control parameters need to be developed for reproducibility across batches. Correlation of physicochemical properties (phase composition, crystallite size) with pharmacological activity and clinical outcomes is essential. Additionally, large-scale toxicity, bioavailability, and clinical studies are required to establish global acceptance and regulatory approval of herbo-mineral formulations.

Research Gap

Despite extensive XRD-based studies, there is a lack of standardized methodologies and reference databases for Ayurvedic Bhasmas. Limited correlation exists between XRD findings and biological efficacy or clinical validation. Variability in preparation methods leads to inconsistent phase composition and particle size, affecting reproducibility. Moreover, insufficient data is available on long-term toxicity, pharmacokinetics, and interaction with biological systems, highlighting the need for interdisciplinary and evidence-based research approaches.

DISCUSSION

X-ray diffraction (XRD) analysis demonstrates that Ayurvedic processing techniques induce significant physicochemical transformations, evidenced by the conversion of elemental metals into stable oxide and sulfide phases. The absence of metallic peaks confirms effective detoxification, while peak broadening indicates reduced crystallite size and possible nanocrystalline formation, which may enhance bioavailability.

Consistent diffraction patterns reflect structural stability of properly prepared Bhasmas; however, observed variability highlights the influence of preparation methods and the need for standardization. In herbo-mineral formulations, the formation of multi-phase crystalline systems further supports complete transformation and integration of constituents.

Although XRD provides reliable phase identification, its limitations in detecting amorphous content necessitate complementary analytical techniques. Overall, XRD findings offer strong scientific validation for traditional Ayurvedic formulations and their therapeutic potential.

REFERENCES

1. Rengarajan K. Analytical Study (XRD, XRF, EDXRF & PSA) on Tarakeswara Rasa - A Herbo-Mineral Preparation. *Int J Health Sci Res*, 2023; 13(8): 27-34. doi:10.52403/ijhsr.20230805
2. Dhamal, S., X-ray Diffraction study for chemical analysis of Rajat based bhasmas. International Journal of Ayurvedic Medicine, 2022; 13(4): 891–895. International Journal of Ayurvedic Medicine. http://ijam.co.in
3. Gupta R, Lakshmi V, Jha C. X-Ray Diffraction of different samples of Swarna Makshika Bhasma. *AYU (An international quarterly journal of research in Ayurveda)*, 2015; 36(2): 225. doi:10.4103/0974-8520.175547
4. Reddy KS, Reddy DrS. X-ray diffraction: A non-destructive technique for crystalline structure analysis. *International Journal of Chemical Research and Development*, 2025; 7(1): 63-66. doi:10.33545/26646552.2025.v7.i1a.81
5. Ali A, Chiang YW, Santos RM. X-Ray Diffraction Techniques for Mineral Characterization: A Review for Engineers of the Fundamentals, Applications, and Research Directions. *Minerals*, 2022; 12(2). doi:10.3390/min12020205
6. Vadalkar VP, Sathe DrN. Corresponding XRF, XRD and FTIR analysis of Hirak Bhasma prepared as per Ayurved Prakash. *J Pharmacogn Phytochem*, 2024; 13(5): 160-170. doi:10.22271/phyto.2024.v13.i5b.15069
7. Rajurkar N, Kale B, Kantak S. *Synthesis and Characterization of Mandur Bhasma*. Vol 6. 2015. www.ijpba.info
8. Kantak S, Rajurkar N, Adhyapak P. Synthesis and characterization of Abhraka (mica) bhasma by two different methods. *J Ayurveda Integr Med*, 2020; 11(3): 236-242. doi:10.1016/j.jaim.2018.11.003
9. Rudramma Hiremath CBJKKN. Vanga Bhasma and Its XRD Analysis. *Anc Sci Life*, 2010; 29(4): 24-28.
10. Singh RK, Kumar S, Aman AK, Karim SM, Kumar S, Kar M. Study on physical properties of Ayurvedic nanocrystalline Tamra Bhasma by employing modern scientific tools. *J Ayurveda Integr Med*, 2019; 10(2): 88-93. doi:10.1016/j.jaim.2017.06.012
11. Reddy KRC, Bhargava S, Sastry GVS. Identifications studies of Lauha Bhasma by X-ray diffraction and X-ray fluorescence. *AYU (An International Quarterly Journal of Research in Ayurveda)*, 2012; 33(1): 143. doi:10.4103/0974-8520.100332
12. Pareek A, Bhatnagar N. Physico-chemical characterization of traditionally prepared Yashada bhasma. *J Ayurveda Integr Med*, 2020; 11(3): 228-235. doi:10.1016/j.jaim.2018.11.004
13. Gandhi I, Bhargava VP, Sharma P. *Antioxidant and Toxicological Evaluation of Cassia Sophera in Streptozotocin Induced Diabetic Wistar Rats. View Project Aashish Netam*, 2021. https://www.researchgate.net/publication/356001919
14. Khedekar S, Bedarkar P, Prajapati P. Physicochemical characterization of Shadguna Balijarita Makaradhwaja: A preliminary study. *AYU (An international quarterly journal of research in Ayurveda)*, 2016; 37(3): 230. doi:10.4103/ayu.ayu_126_15
15. Srikanth N, Singh A, Ota S, Sreedhar B, Galib, Dhiman KS. Chemical characterization of an Ayurvedic herbo-mineral preparation-Mahalaxmivilas Rasa. *J Ayurveda Integr Med*, 2019; 10(4): 262-268. doi:10.1016/j.jaim.2018.01.002
16. Ota S, Singh A, Srikanth N, Sreedhar B, Ruknuddin G, Dhiman K. Chemical characterization of an Ayurvedic herbo-mineral formulation - Vasantakusumākara Rasa: A potential tool for quality assurance. *Anc Sci Life*, 2017; 36(4): 207. doi:10.4103/asl.asl_66_17
17. Rasheed A, Naik M, Pillanayil K, et al. *Formulation, Characterization and Comparative Evaluation of Trivanga Bhasma: A Herbo-Mineral Indian Traditional Medicine*. Vol 27. 2014.
18. Meher L and DAK. Structural and Chemical Characterization of Rasaparpati w.s.r to X-ray Diffraction. *Indian Journal of Ayurveda and Research*, 2018; 1: 51-54.
19. Jagtap CY, Mishra AK, Nariya M, Shukla VJ, Prajapati PK. Product development and characterization of the Ayurvedic herbo-mineral-metallic compound- Hridayarnava Rasa. *J Ayurveda Integr Med*, 2024; 15(3). doi:10.1016/j.jaim.2024.100886