

X-ray Diffractometric and Elemental Analysis of Sialolith, Dental Calculus and Odontome

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ABSTRACT

We are living in a world of rapid change and technology which is increasingly used in medical practice, has increased our confidence in solving specific problems. Technology that serves the patient better rejuvenates the clinical and diagnostic accuracy.

Keywords: X-ray diffraction, Sialolith, Calculus, Odontome, Hydroxylapatite.

INTRODUCTION

We are living in a world of rapid change and technology which is increasingly used in medical practice. Supragingival or subgingival calculus is an adherent calcified or calcifying mass that forms on the surface of natural teeth. Whereas sialolith is the occurrence of calcareous concretions in the salivary ducts or glands. They are more common in submandibular gland due to the tenacity of its secretion. Odontome is any tumor of odontogenic origin. They can be divided into two types; compound composite and complex composite odontome.¹

AIMS AND OBJECTIVES

To use X-ray diffraction (XRD) is to know the basic inorganic chemical composition of the calcification and to compare the chemical composition between normal and pathologic calcification which will add to our knowledge of the underlying pathologic process.

X-RAY DIFFRACTION

German physicist, Von Laue,² in 1912 reasoned that crystals composed of regularly spaced atoms may act as scattering centers for X-rays and they could be diffracted by crystals. The first experiment was carried out with crystals of copper sulfate and formed a pattern of spots on the photographic plates. WH Bragg and WL Bragg,¹ English physicists, successfully analyzed Laue's experiment and were able to give diffraction in simple mathematical form. They solved the structure of NaCl, KCl, KBr, KI and were the first complete crystal structure determinations ever made.

MATERIALS AND METHODS

The specimens of the study consisted of four sialoliths, two supragingival and subgingival calculus and three odontoma.

1. *X-ray diffraction method:* Two types of X-ray diffraction analysis were carried out. There are as follows:
 - a. X-ray diffraction by using computerized scanning method: This analysis was carried out at RSIC, Nagpur University on Philips (Holland) automated XRD.
 - b. X-ray diffraction analysis using radiographic plate technique or Debye-Scherrer method: This analysis was carried out in physical laboratory of MECL, Nagpur. In this study, a four window Philips X-ray tube with iron target is fitted to the generator.
2. *Spectrochemical analysis or elemental analysis:* This was also carried out at physical laboratory of MECL Nagpur. This is based on the principle that each element emits its own characteristic radiant energy or light and on wavelength measurement of the component lines of its spectrum enable to ascertain which elements are present.

DISCUSSION

Sialolith

In the present study, hydroxylapatite $\text{Ca}_3(\text{PO}_4)_3\cdot\text{OH}$ is the only phase detected in computerized analysis. By Debye-Scherrer method, calcite was detected in all the samples (Table 1).

Anneroth,¹ Blatt et al (1975) showed that main component of the sample was apatite on the basis of microdiffraction analysis.

Sakae T, Yamamoto H et al^{1,3} (1979), Mishima H, Yamamoto H⁴ (1992) reported that hydroxylapatite, octacalcium phosphate,

Table 1: Master chart

S.No.	Sample	RSIC(XRD) analysis	MECL analysis	Elemental analysis
1.	1 Sialolith	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂ Traces: Ca ₂ Mg(PO ₄) ₂ ·2H ₂ O	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
2.	2 Sialolith	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂ Traces: Ca ₂ Mg(PO ₄) ₂ ·2H ₂ O	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
3.	3 Sialolith	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂ Traces: Mg ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
4.	4 Sialolith		Ca ₃ (PO ₄) ₂ Traces: Mg ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
5.	Supragingival calculus 1	Antarcticite 1-1220 CaCl ₂ ·6H ₂ O	Ca ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg
6.	Supragingival calculus 2	Whitlockite 9-169 Ca ₃ (PO ₄) ₂	Ca ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
7.	Subgingival calculus 1	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
8.	Subgingival calculus 2	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg Traces: K, Fe
9.	1 Odontome	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂	Major: Ca, Mg Traces: K, Fe, Na
10.	2 Odontome	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂	Major: Ca, Mg Traces: K, Fe, Na
11.	3 Odontome	Hydroxylapatite 9-432 Ca ₃ (PO ₄) ₃ -OH	Ca ₃ (PO ₄) ₂	Major: Ca Minor: Na, Si, Mg Traces: K, Fe

whitlockite, trishite, weddellite and calcite have been reported as the crystalline phase of salivary stones.

Bursteln⁵ et al (1979) noted that hydroxylapatite and magnesium substituted whitlockite are co-phases in salivary stones of submandibular gland origin.

Yamamoto, Sakae^{3,6} et al (1981) revealed using XRD that apatite is the primary phase in salivary calculi. In some calculi, whitlockite, brushite and octacalcium phosphate are also present.

Oguzcan Kasaboglu⁷ et al (2004) noted that the sialolith contained hydroxylapatite crystal in their study.

Presence of hydroxylapatite and calcium phosphate hydrated and calcite are detected and these findings are in agreement with previous studies.

Dental Calculus

XRD analysis of two supragingival calculus at RSIC shows presence of antarcticite as the major phase in one sample CaCl₂·H₂O, while in other sample, whitlockite Ca₃(PO₄)₂ is the primary phase (see Table 1). And XRD analysis at MECL reveals the presence of calcium phosphate [Ca₃(PO₄)₂] is the major phase detected in both samples (see Table 1).

In the subgingival calculus samples, both the samples on XRD analysis at RSIC show presence of hydroxylapatite Ca₃(PO₄)₃-OH as the major phase (see Table 1). The analysis at MECL reported calcium phosphate Ca₃(PO₄)₂ as the major phase (see Table 1).

Jensen⁸ et al (1954) suggested that based on XRD data hydroxyapatite, whitlockite, and brushite are common constituents of calculus. Whitlockite is abundant in subgingival calculus, whereas brushite is abundant in supragingival calculus attached to the mandibular anterior teeth.

Jensen⁸ et al (1957) proved the presence of magnesium whitlockite as a major constituent of dental calculus as well as the presence of tetracalcium hydrogen, triphosphate and trihydrate.

Groan⁸ et al (1967) demonstrated that octacalcium phosphate is found least frequently in posterior supragingival calculus and whitlockite is found most abundantly in subgingival calculus.

Kani T, Kani M⁹ (1983) in their study noted that hydroxyapatite (HA) and octacalcium phosphate (OCP) were frequently found in deposits in the porous and zonal structure. In a deposit having an homogeneous structure with high calcification, whitlockite (WL) was most abundant, along with a minor component of brushite (Bru) with low crystallinity.

Ogino⁸ et al (1983) reported whitlockite was chiefly detected in supragingival calculus.

Sundberg⁸ et al (1985) described platelet like shapes of octacalcium phosphate crystals and needle-shaped hydroxylapatite crystals in supragingival calculus and bulk crystals of whitlockite is predominant component in subgingival calculus.

Yamamoto⁸ et al (1988) reported apatite as the major phase in supragingival calculus. Coexistence of hydroxylapatite and whitlockite was more common in subgingival calculus.

The finding of whitlockite in one sample of supragingival calculus is in agreement with Ogino et al but not in agreement with Sundberg et al, Yamamoto et al, Groan et al and Jensen et al.

Hayashizaki¹⁰ et al (2008) carried in his study of site specific mineral composition of human supragingival calculus, the crystalline content of the calculus formed on upper molar is higher than formed on lower anteriors.

The finding of antarcticite in other sample is not in agreement with the previous studies.

The finding of hydroxylapatite in both samples of subgingival calculus is in agreement with the studies of Yamamoto¹¹ et al. But the absence of whitlockite in subgingival calculus is in contrast to the studies of Sundenberg et al, Jensen et al and Groan et al.

Odontomes

In the present study, hydroxylapatite was detected as the primary phase in all three samples of odontomas on XRD analysis (see Table 1). On elemental analysis of two samples, calcium and magnesium are the major element. Elemental analysis of the remaining sample shows that magnesium is a minor element and calcium is the major element.

Aoba¹¹ et al (1980) reported on XRD analysis of five samples that apatite pattern characteristic of enamel structure is visualized. The B2 values of the crystals in the lesions are greater than those of normal apatites. This indicates crystals are smaller in size and or have more lattice defects.

Eachara¹¹ and Fischer et al (1969) established that magnesium can reduce the rate of mineral deposition and inhibit apatite formation.

Suga¹¹ et al (1971) found elevation of magnesium concentration across the hypomineralized areas.

Robinson¹¹ et al (1979) pointed that odontomes contain higher magnesium concentration, which is associated with organic phase. So, increased level of magnesium may be ascribed to disorder of process of matrix formation.

The finding of hydroxylapatite as the major phase in odontomes and a high concentration of magnesium in odontomes (major phase) is in agreement with the previous studies.

CONCLUSION

In view of the observations from these 11 samples following conclusions can be drawn: X-ray diffraction analysis shows that calcium phosphate (hydroxylapatite) is the chief constituent of sialolith. XRD analysis detected antarcticite and whitlockite in supragingival calculus. XRD analysis detected hydroxylapatite as the main constituent in subgingival calculus. Odontome XRD analysis shows presence of hydroxylapatite. Magnesium content of odontome is more on elemental analysis. To substantiate these findings, more studies are advised.

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