

H102 Preliminary Validation of Handheld X-Ray Fluorescence (HHXRF) Spectrometry for Distinguishing Osseous and Dental Tissue From Non-Bone Material of Similar Chemical Composition

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After attending this presentation, attendees will have a better understanding of the benefits of utilizing Handheld X-ray Fluorescence (HHXRF) spectrometry and statistical analysis to distinguish fragmentary osseous and dental material from non-bone material of similar chemical composition.

This presentation will impact the forensic science community by demonstrating that the HHXRF is a valid method for distinguishing between fragmentary osseous or dental material and non-bone material of similar chemical composition in a laboratory setting.

Identifying bone and osseous material that is highly fragmented, burned/charred, and subjected to extensive taphonomic processes can be difficult based on the poor quality of the bone. In most cases, bone and non-bone fragmentary materials are sorted in the field using gross methods; however, in cases involving indeterminate fragments, other methods may be used to sort the material in a laboratory setting. Current laboratory methods include histological analysis and chemical methods determining elemental composition. A recent chemical method proposed by Ubelaker et al. (2002) involves the use of Scanning Electron Microscopy and Energy-Dispersive X-ray Spectroscopy (SEM/EDS).¹ This method provides the Ca/P ratios of analyzed materials, and allows for the formation of a spectral library. More recently, X-ray Fluorescence (XRF) spectrometry, which analyzes the chemical composition of small, fragmentary specimens, and then allows for the specimens to be sorted based on Ca/P ratios, was proposed as a viable method.² HHXRF instruments have recently come into use in areas of criminal justice and physical anthropology.

The purpose of this research was to determine the applicability of using an HHXRF for discriminating non-bone material (including material with a similar composition to bone) from osseous and dental material using statistical methods for discrimination purposes.

A total of 28 samples were analyzed, with three spectra taken from different locations on each sample. Samples consisted of human and non-human bones (archaeological, anatomical), non-biological specimens (rock phosphate, rock apatite, synthetic hydroxyapatite, plastic, glass), and other biological specimens (sand dollar, three shell species, two coral species, turkey spurs, bark). A Bruker Elemental S1 Turbo-SDR HHXRF unit was used with upgraded analytical software, S1PXRF (provided by the manufacturer), which allowed for the detection of low-mass elements. The HHXRF was mounted on a vertical stand for stationary analysis and samples were placed directly onto the examination window for analysis using a 15 kV/Filter 2. Post-processing of the data involved removing calcium from the spectrum and normalizing the integrated area of the remaining trace elements, Principle Component Analysis (PCA) using MatLab version 2011b by Mathworks, and Linear Discriminant Analysis (LDA) based on principle components representing 95% of the variance in the data using SYStat version 13 by Cranes Software International.

Initial analyses indicated that cleaning may be required when soil staining is involved, as a number of dental specimens were discriminated from non-bone samples only after minimal processing with a Dremel tool. Results of the LDA showed 97% average discrimination between bone and non-bone samples (with 2% of bone samples misclassifying as non-bone and 5% of non-bone misclassifying as bone). The samples that misclassified were rock apatite, synthetic hydroxyapatite, and an alligator rib bone. The misclassification was a result of only one out of the three collected spectra per sample, as the other two spectra were correctly classified for these specimens. Statistical methods are being examined to remove possible outliers in the data.

The combination of an HHXRF with statistical analysis shows promise for discriminating fragmentary osseous and dental tissue from other types of material, due to the analysis of all detected elements after removal of calcium from the spectrum and normalization of the integrated area of the remaining trace elements. Further research will explore the application of this method by expanding the sample size and determining which location on the bone offers the most accurate discrimination, as well as the applicability of this method to the field in the form of the establishment of a bone library on the HHXRF.

References:

- ^{1.} Ubelaker DH, Ward DC, Braz VS, Stewart J. The use of SEM/EDS analysis to distinguish dental and osseus tissue from other materials. *J Forensic Sci* 2002;47(5):1-4.
- ². Christensen AM, Smith MA, Thomas RM. Validation of X-ray fluorescence spectrometry for determining osseous or dental origin of unknown material. *J Forensic Sci* 2012;57(1):47-51.

Forensic Science, X-Ray Fluorescence, Elemental Analysis

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