A MACHINE LEARNING APPROACH TO INVESTIGATE THE MATERIALS SCIENCE OF AGING ENAMEL

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Introduction

Understanding aging of tooth tissues is critical to patient-centric oral healthcare. Traditional methods for analyzing the composition-structure-property relationships of hard tissues are not robust enough for the complex multi-dimensional aspects of aging. We implement self-organizing maps (SOMs) algorithms to gain new insights into the aging of enamel. We hypothesize SOMs will reveal unique correlations not yet established by traditional methods.

Objective

To apply unsupervised machine learning techniques to assess the complex composition-structure-property relationships between teeth from donors of three different age groups.

Methods

- Extracted human non-carious vital teeth (N = 22)) were obtained with approved protocol and divided into young (age ≤ 8, n=7) , adult (24 ≤ age ≤ 46, n=7) , and old (age ≥ 55, n=8) groups.
- The teeth were sectioned buccal-lingually and polished to mirror finish using traditional methods. Nanoindentation was used to characterize the elastic modulus and hardness as a function of distance from the dentin-enamel junction (DEJ).
- A co-located analysis of the chemical composition and mineralogic structure was performed using Raman spectroscopy mapping (**Fig. 1**).
- SOMs were implemented to identify the multi-dimensional composition-structure-property relationships of each age group.

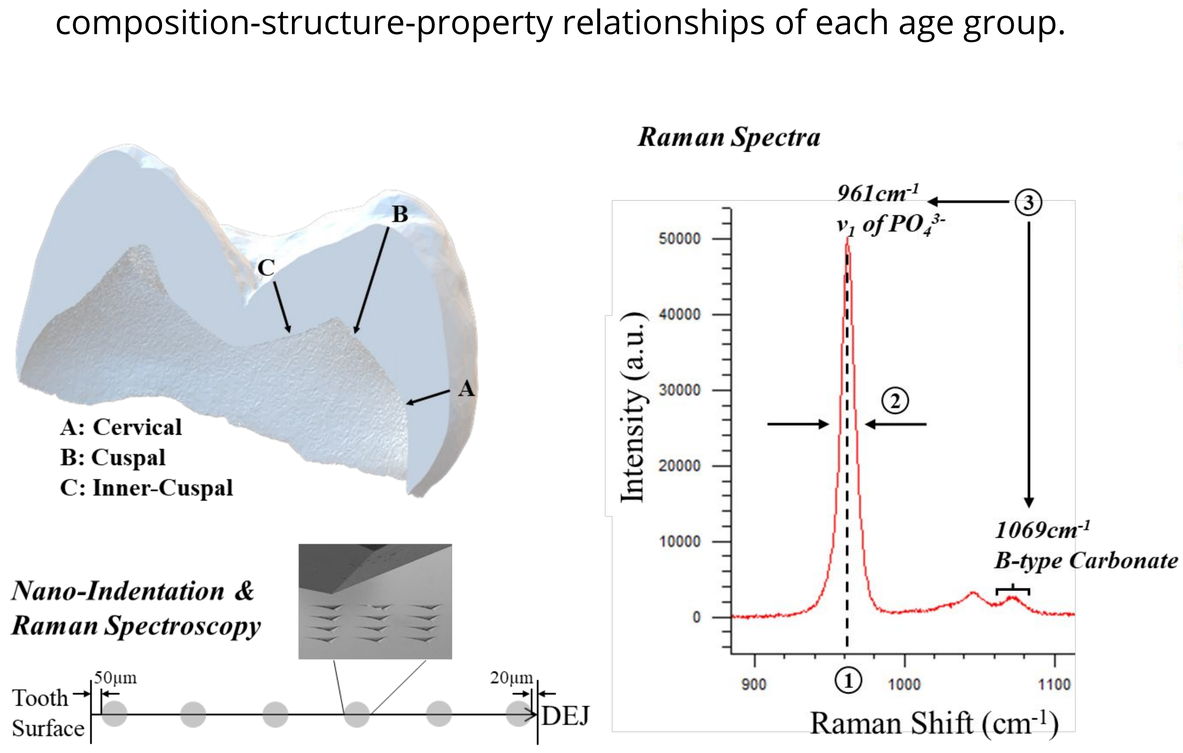

Figure 1 Bucco-lingual sectioning followed by subsequent polishing was performed and the co-located nanoindentation and Raman were conducted along three trajectories including cervical, cuspal and inner-cuspal locations. The Raman spectra were analyzed to quantify the site-specific composition.

Results

- The elastic modulus and hardness increase significantly ($P < 0.05$) with age. These properties also increase significantly ($P < 0.05$) from the DEJ to the enamel surface for all ages (**Fig. 2**).
- Raman spectra showed increasing crystallinity and fluoridation from the DEJ to the outer enamel surface for all age groups (**Fig. 3**). Values for the outer enamel of primary teeth are significantly ($P < 0.05$) lower at surface.
- The mechanical properties are positively correlated with crystallinity and fluoridation as a function of distance from the DEJ to the outer enamel surface. The opposite trend is seen for the carbonate substitution.
- The SOMs supported pooling of spatial data within the three regions of enamel and revealed a non-linear aging process. The old enamel SOMs exhibit a unique clustering pattern (**Fig. 4**) as a result of the aging processes that involves fluoridation and warrants further study.

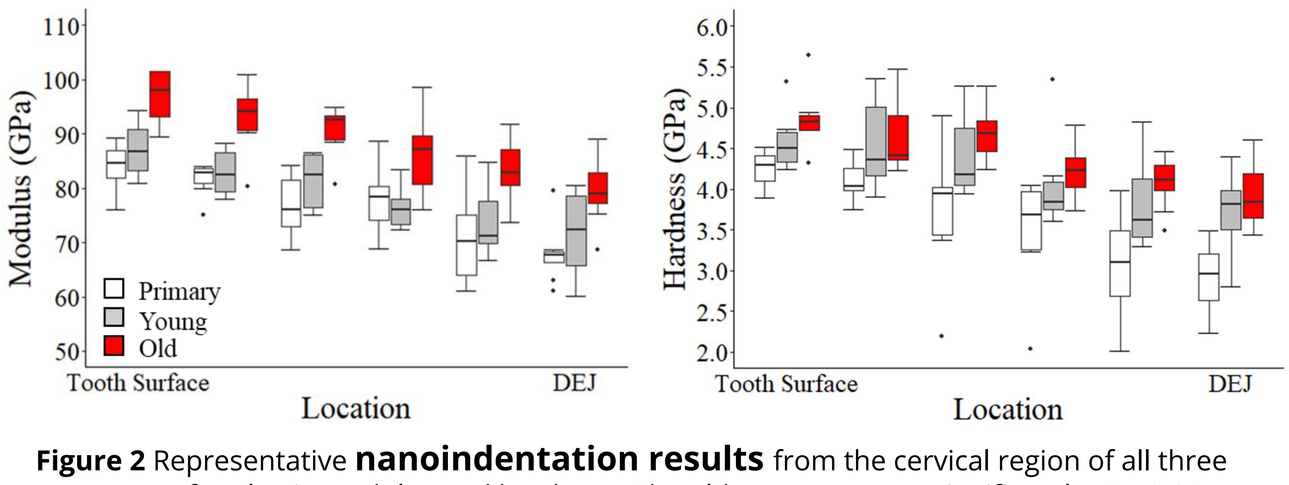

Figure 2 Representative **nanoindentation results** from the cervical region of all three age groups for elastic modulus and hardness. The old age group was significantly ($P < 0.05$) more stiff and harder than the two other age groups.

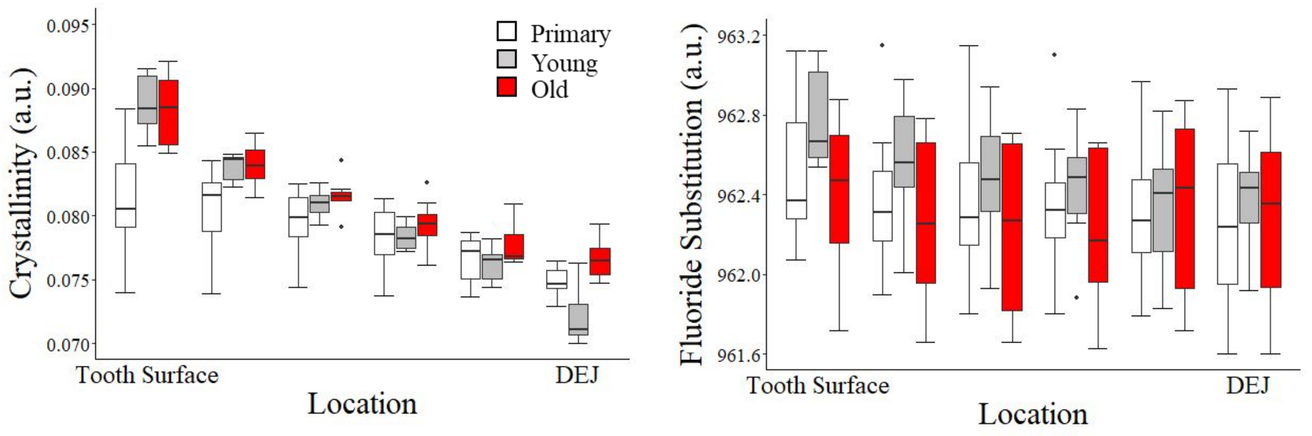

Figure 3 Representative **Raman spectroscopic results** from the cervical region of all three age groups for crystallinity (FWHM) and fluoride substitution. Carbonate substitution is not displayed but showed the opposite trend with no differences between age groups.

Conclusion

Based on the findings, unsupervised machine learning methods can reveal complex non-linear composition-structure-property relationships in tooth tissues and will help to understand the materials science of aging.

SOMs Cluster Maps (Unsupervised Machine Learning)

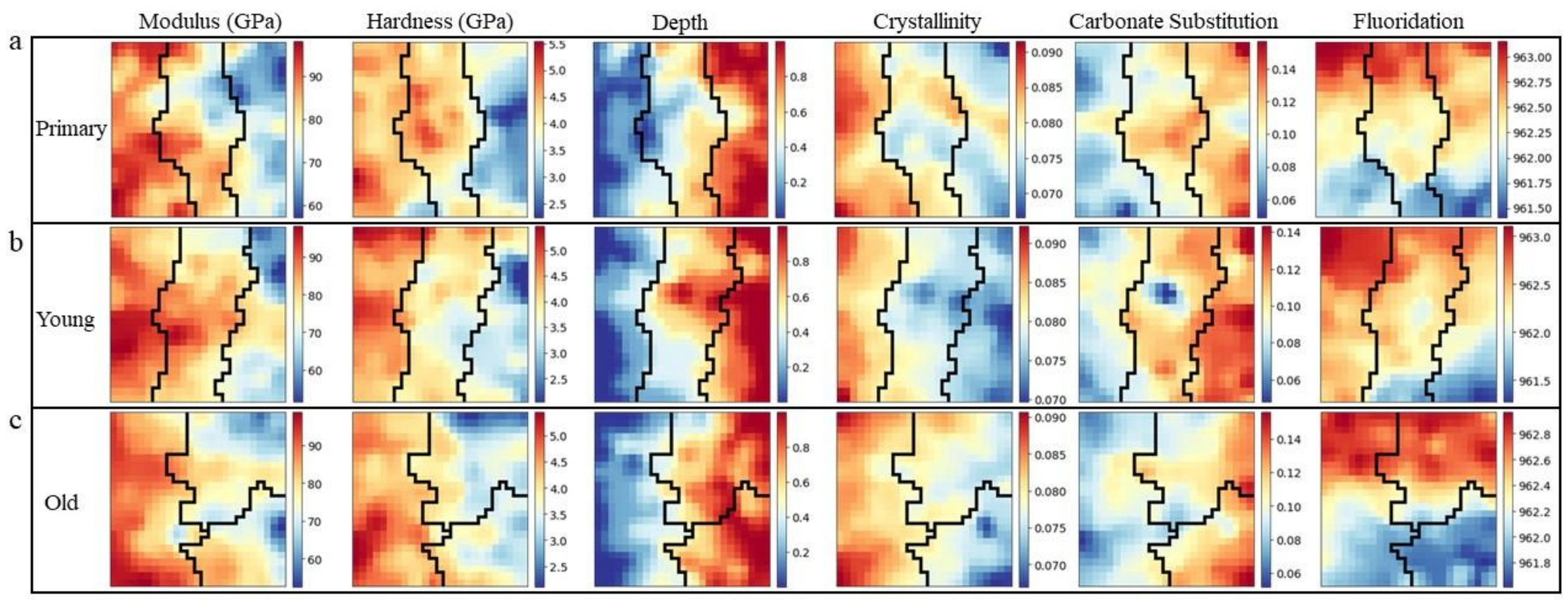

Figure 4 Heat maps for modulus. hardness, depth, crystallinity, carbonate substitution and fluoridation. Individual maps are presented for the primary, young and old age groups. The primary and young enamel are clustered predominately by depth. The old group does not show the same clustering pattern due to the unique influence of fluoride that develops.

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