Submission Date: 06/10/2025

2024 Academic Year Bio-SPMs Collaborative Research
Research Report Summary

Title of the research project		Molecular structure of the amelogenin nanoribbons-water interface and its role in directing mineralization	
PI (Person in charge of the research project)	Name	Dr. James De Yoreo	
	Affiliated Institution and Department/Division/etc.	Pacific Northwest National Laboratory Physical and Computational Sciences	
	Position	Battelle Fellow	
Bio-SPMs that you used (Check the boxes)		✔	Atomic resolution/3D-AFM
		☐	High-speed AFM
		☐	SICM
		☐	AFM for Cell Measurement
Collaborative NanoLSI Faculty Members		Dr. Ayhan Yurtsever	

Tooth enamel's extraordinary hardness is attributed to the well-organized architecture of the hydroxyapatite (HAP), a calcium phosphate mineral. Prior studies suggest that amelogenin-derived nanoribbons (Amel NRs), which exhibit amyloid-like, co-aligned structures, act as scaffolds that facilitate the transformation of amorphous calcium phosphate (ACP) into crystalline HAP. This transformation is believed to be guided by the stereochemical and energetic compatibility between the peptides and mineral precursors. This study explores how specific functional domains within amelogenin peptides influence their ability to self-assemble into nanoribbons and guide mineralization. Building on previous kinetic studies, the current work aims to determine the 3D structure of Amel NRs at near-atomic resolution and assess the role of peptide domains in organizing precursor ions and, thus, templating apatite formation.

High-resolution and 3D atomic force microscopy (HR-AFM and 3D-AFM) were employed to study the structures of the Amel-NR and overlying hydration layers with the goal of relating peptide structure to the outcome of self-assembly and organization of water. The results indicate that peptide-peptide and peptide-surface interactions depend on head-group chemistry and are critical to ribbon organization. Atomic-resolution imaging also shows that phosphorylation at the serine terminus introduces slight changes in nanoribbon assembly, which potentially correlates with differences in ACP nucleation rates between the unmodified 14P2 peptide and its phosphorylated version, p14P2.

3D-AFM imaging of the peptide-water interface demonstrated that water is more densely structured over hydrophilic domains of the peptide, and that lower-density regions frequently occur in the zones between adjacent ribbons where they interact laterally. These hydration structures likely influence how calcium and phosphate ions interact with and organize at the NRs. By comparing Δf maps in different orientations and across various ACP concentrations, the study helps ellucidate how ions assemble and eventually mineralize into HAP. These insights will be foundational for developing biomimetic strategies to synthesize enamel-like materials with hierarchical organization at the nano- and microscale.

*This form (Form 3) will be open on the NanoLSI website in the following academic year.

*Note that this form should be prepared in one A4-size paper.

*Submission Deadline: May 9, 2025 (Friday). Submit it as a PDF file.

*Submission Destination: the person in charge of Bio-SPMs collaborative research at WPI-NanoLSI, Kanazawa University