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Matching 4.7-Å XRD Spacing in Amelogenin Nanoribbons and Enamel Matrix

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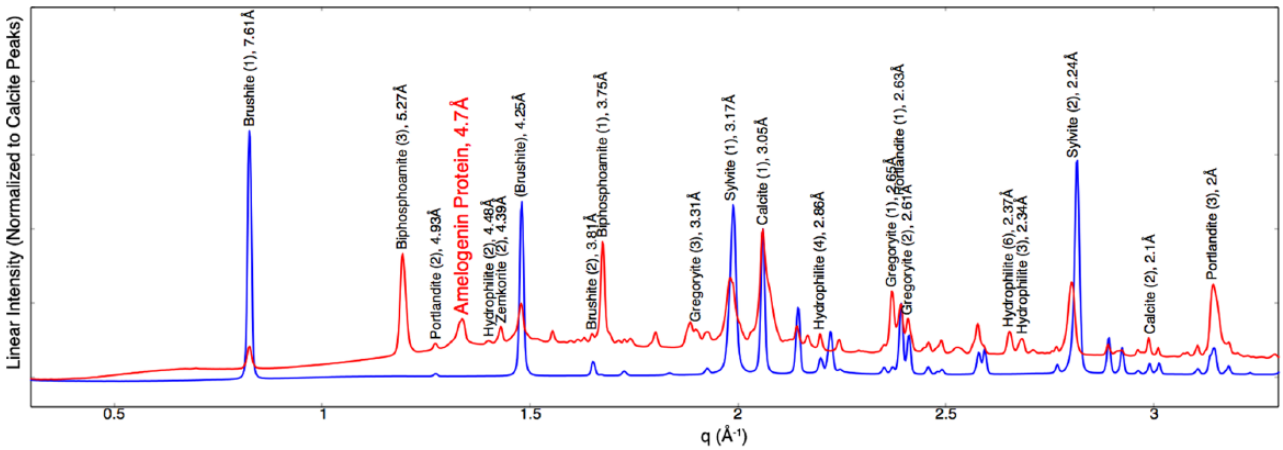
APPENDIX

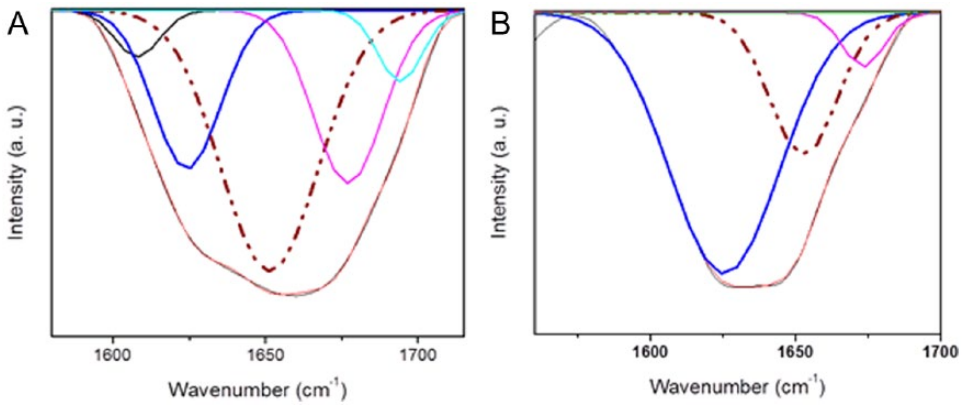
Appendix Table. List of Reflections from XRD Data of Samples with rH174 Nanoribbons and Matching Mineral and Protein Structure Assignments

d spacing (Å)	Intensity (fraction of protein int.)	Present w/o rH174	Mineral Name (#Intensity) (hkl)	Formula
2	0.91	*	Portlandite (3)	$CaOH_2$
2.1	0.39		Calcite (2) (–222)	$CaCO_3$
2.24	1.05	*	Sylvite (2)	KCl
2.34	0.49		Hydrophilite (3)	$CaCl_2$
2.37	0.57		Hydrophilite (6)	$CaCl_2$
2.44	0.62	*	NA	
2.61	0.78	*	Gregoryite (2)	$K_2CO_3/CaCO_3$
2.63	0.92	*	Portlandite (1)	$CaOH_2$
2.65	1.11		Gregoryite (1)	$K_2CO_3/CaCO_3$
2.86	0.56	*	Hydrophilite (4)	$CaCl_2$
2.9	0.61		NA	
2.93	0.73	*	NA	
3.05	2.22	*	Calcite (1) (0-14)	$CaCO_3$
3.17	1.65	*	Sylvite (1)	KCl
3.26	0.71		NA	
3.31	0.76		Gregoryite (3)	$K2CO_3/CaCO_3$
3.49	0.74		NA	
3.6	0.63		NA	
3.64	0.61		NA	
3.66	0.60		NA	
3.75	2.31		Biphosphoamite (1)	KH_2PO_4
3.81	0.70	*	Brushite (2)	$CaHPO_4•2(H_2O)$
3.86	0.65		NA	
3.89	0.62		NA	
3.94	0.60		NA	
3.96	0.59		NA	
4.04	0.77		NA	
4.25	1.22	*	Brushite	$CaHPO_4•2(H_2O)$
4.39	0.87		Zemkorite (2)	$K_2Ca_2(CO_3)_2$
4.48	0.62		Hydrophilite (2)	$CaCl_2$
4.7	1.00		**Amelogenin protein**	**rH174 β-sheets**
4.93	0.59		Portlandite (2)	$CaOH_2$
5.27	2.20		Biphosphoamite (3)	KH_2PO_4
7.61	0.57	*	Brushite (1)	$CaHPO_4•2(H_2O)$

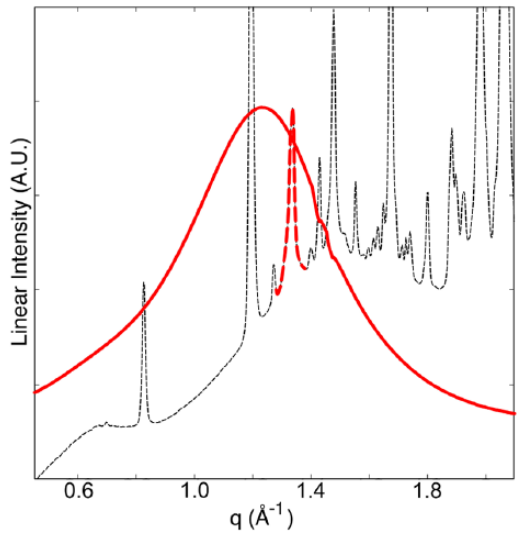
NA = not assigned.



Appendix Figure 1. XRD analysis. Full range of analysis of buffer with amelogenin rH174 (red) and without protein (blue). Mineral precipitates have been indicated with PF4+ files in the International Centre for Diffraction Data (ICDD) databank.



Appendix Figure 2. Deconvolution of FTIR spectra between 1,600 and 1,700 cm^{-1} for **(A)** amelogenin nanospheres and **(B)** amelogenin nanoribbons. Gaussian curves were fitted to the amide-I peak with fixed x-axis positions for each functional group: extended/amyloid at 1,612 cm^{-1} (black); β-sheet at 1,625 cm^{-1}(blue); random coil at 1,650 cm^{-1} (brown and dotted); α-helix at 1,670 cm^{-1} (pink); secondary β-sheet at 1,690 cm^{-1} (light blue); composition spectrum (red); and original spectrum (red). Assignment of secondary structural motifs according to Byler and Susi (1986) and Shivu *et al.* (2013). Proportions of areas under the curves were calculated by Origin 7.5 and Gauss-Curve fitting as described in Beniash *et al.* (2012). Secondary structure content is listed as percentage of total area in the Table in the main paper.



Appendix Figure 3. Powder XRD analysis of the broad peak of the pure lyophilized protein sample (solid red line) in comparison with the sharper peak associated with the protein in the calcium phosphate solution (dashed red line). The rest of the diffraction profile from the calcium phosphate solution is shown as well (dashed black line).

APPENDIX REFERENCES

Beniash E, Simmer JP, Margolis HC (2012). Structural changes in amelogenin upon self-assembly and mineral interactions. *J Dent Res* 91:967-972.

Byler DM, Susi H (1986). Examination of the secondary structure of proteins by deconvolved FTIR spectra. *Biopolymers* 25:469-487.

Shivu B, Seshadri S, Li J, Oberg KA, Uversky VN, Fink AL (2013). Distinct beta-sheet structure in protein aggregates determined by ATR-FTIR spectroscopy. *Biochemistry* 52:5176-5183.