

Supporting Information

Size of silk fibroin β -sheet domains affected by Ca^{2+}

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Table S1: Mass spectrometric analysis of sericin in the silk fibroin preparation. Silk sericin extract and fibroin preparation in depicted amounts were hydrolysed in solution with trypsin. Peptide mixtures were analysed on ESI ion trap mass spectrometer 1200 series HPLC-Chip-LC/MSD Trap XCT Ultra. Identification of proteins relies on the MS/MS-derived peptide sequences that are listed.

Sample	Quantity analysed [µg]	Identified proteins	Swiss-Prot accession number	Mascot protein score	Peptide sequence	z	Calculated peptide mass		
silk sericin extract	0.175	sericin 1	SERI1_BOMMO	135	ASSTIYADKDQIR	2	1467.7445		
					ASSTIYADKDQIR	3	1467.7445		
					YTSGPEGVSYSGR	3	1359.6181		
		fibroin light chain	FIBL_BOMMO	110	SIAILNVQEILK	2	1340.8155		
					YIAQAASQVHV	2	1186.6220		
					ASSTIYADKDQIR	2	1467.7445		
	0.35	sericin 1	SERI1_BOMMO	239	KASSTIYADKDQIR	3	1595.8394		
					SDAASEDGFWWW NR	2	1813.7570		
					YTSGPEGVSYSGR	2	1359.6181		
		fibroin light chain	FIBL_BOMMO	200	AWDYVDDTDKSIAIL NVQEILK	3	2549.3143		
					SIAILNVQEILK	2	1340.8155		
					YIAQAASQVHV	2	1186.6220		
fibroin heavy chain	FIBH_BOMMO	52	DASGAVIEEQITTK	2	1460.7358				
			1.75	sericin 1	SERI1_BOMMO	194	NDNVFVYR	2	1026.5008
							SDAASEDGFWWW NR	2	1813.7570
SDAASEDGFWWW NRRK	3	2097.9532							
fibroin light chain	FIBL_BOMMO	153		AWDYVDDTDKSIAIL NVQEILK	3	2549.3143			
				SIAILNVQEILK	2	1340.8155			
				YIAQAASQVHV	2	1186.6220			
fibroin heavy chain	FIBH_BOMMO	72	DASGAVIEEQITTK	2	1460.7358				
			silk fibroin	35	FIBL_BOMMO	123	SIAILNVQEILK	2	1340.8155
							YIAQAASQVHV	2	1186.6220
fibroin heavy chain	FIBH_BOMMO	64					DASGAVIEEQITTK	2	1460.7358

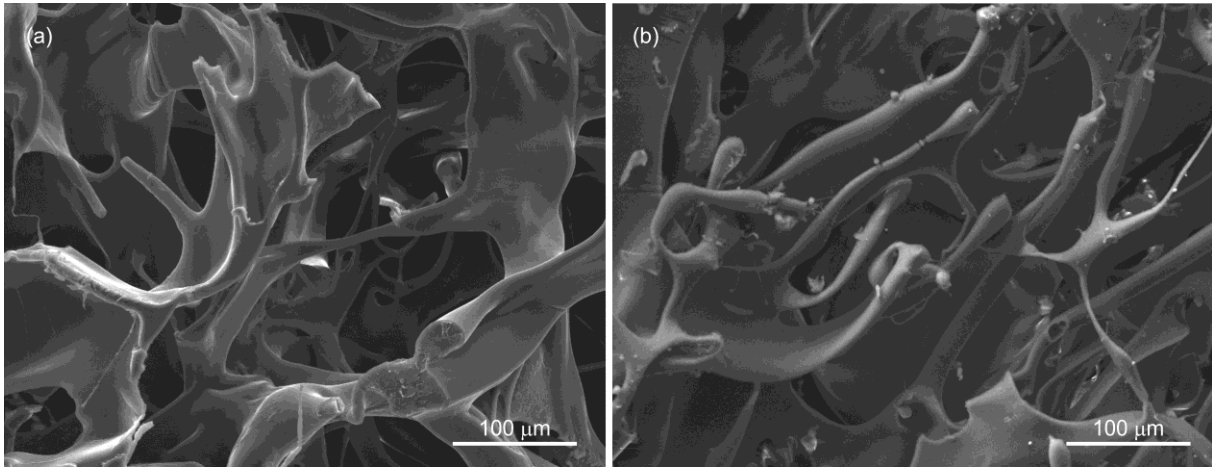


Fig. S1 Microstructures of dried SF scaffolds with the highest concentration of CaCl_2 : (a) Ca300 and (b) Ca500. Threads were formed instead of walls resulting in destruction of the scaffolds during ethanol incubation.

Table S2 The secondary structure peak assignments for amide I band frequencies.

Wavelength (cm^{-1})	Type of secondary structure	Ref.
1715	β -turns	1
1697-1703	β -sheet (weak)	2
1686-1696	β -turns and bends	2
1681-1696	β -turns and bends	3
1671-1685	β -turns and bends	2
1671-1679	β -turns and bends	3
1668-1671	β -turns and bends	3
1663-1670	β -turns and bends	2
1656-1662	α -helices	2
1655	α -helices	4
1654	Random coil	5
1650	Random coil	4
1647-1655	Random coil	2
1641-1647	Random coil	4
1640-1648	Random coil	3
1638-1646	Random coil random coils/extended chains	2, 6
1638	Random coil	5
1628-1637	β -sheets	2-4, 7

1623	Antiparallel β -sheet	2
1621-1627	β -sheet	2, 3
1620	Parallel β -sheet	2
1618	β -sheet	8
1616-1637	β -sheet	9
1616-1621	Aggregate b strand/ β -sheet weak	10
1605-1615	(Tyr) side chains aggregated strands	10

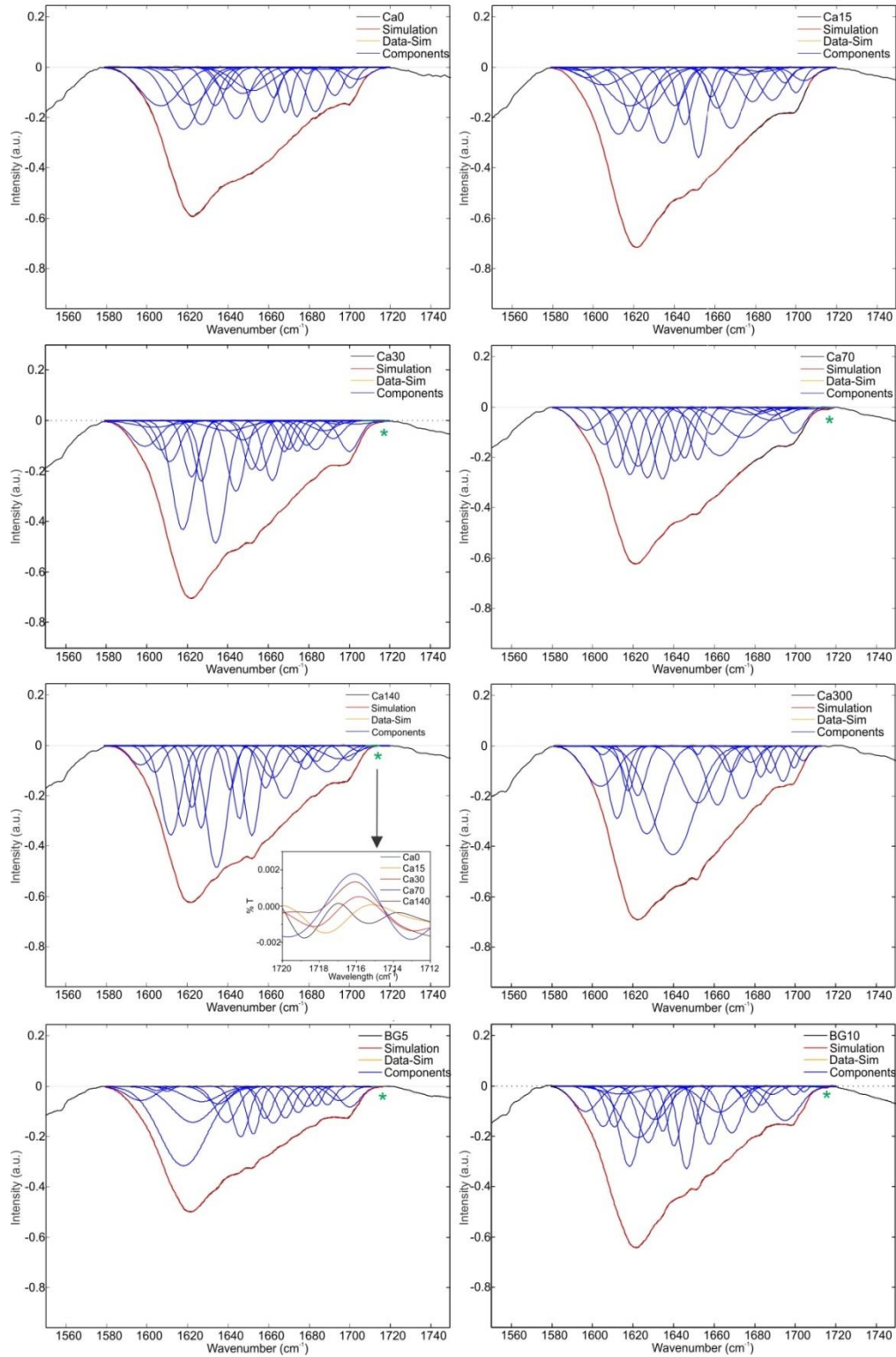


Fig. S2 Fitted amide I band of fibroin scaffolds: Ca0, Ca15, Ca30, Ca70, Ca140, Ca300, BG5 and BG10. New peak arising at around 1715 cm^{-1} is marked with green * and is more clearly presented in the inset in Graph Ca140 that shows second derivative FTIR spectra at wavelengths around 1715 cm^{-1} where the peak representing β -turns increases with Ca concentration.

References

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