Supporting Information (SI)

Grain Structure–Controlled Growth of InSb Crystals: a Grain Boundary Engineering Approach for Enhanced Thermoelectric Performance

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1. Morphological and elemental compositional investigation of the prepared InSb Ingots.

Fig. S1 (a_1-c_3) shows the FESEM images of the prepared ingots SC InSb (a_1-a_3), AQ InSb (b_1-b_3), and IWQ InSb (c_1-c_3) samples.

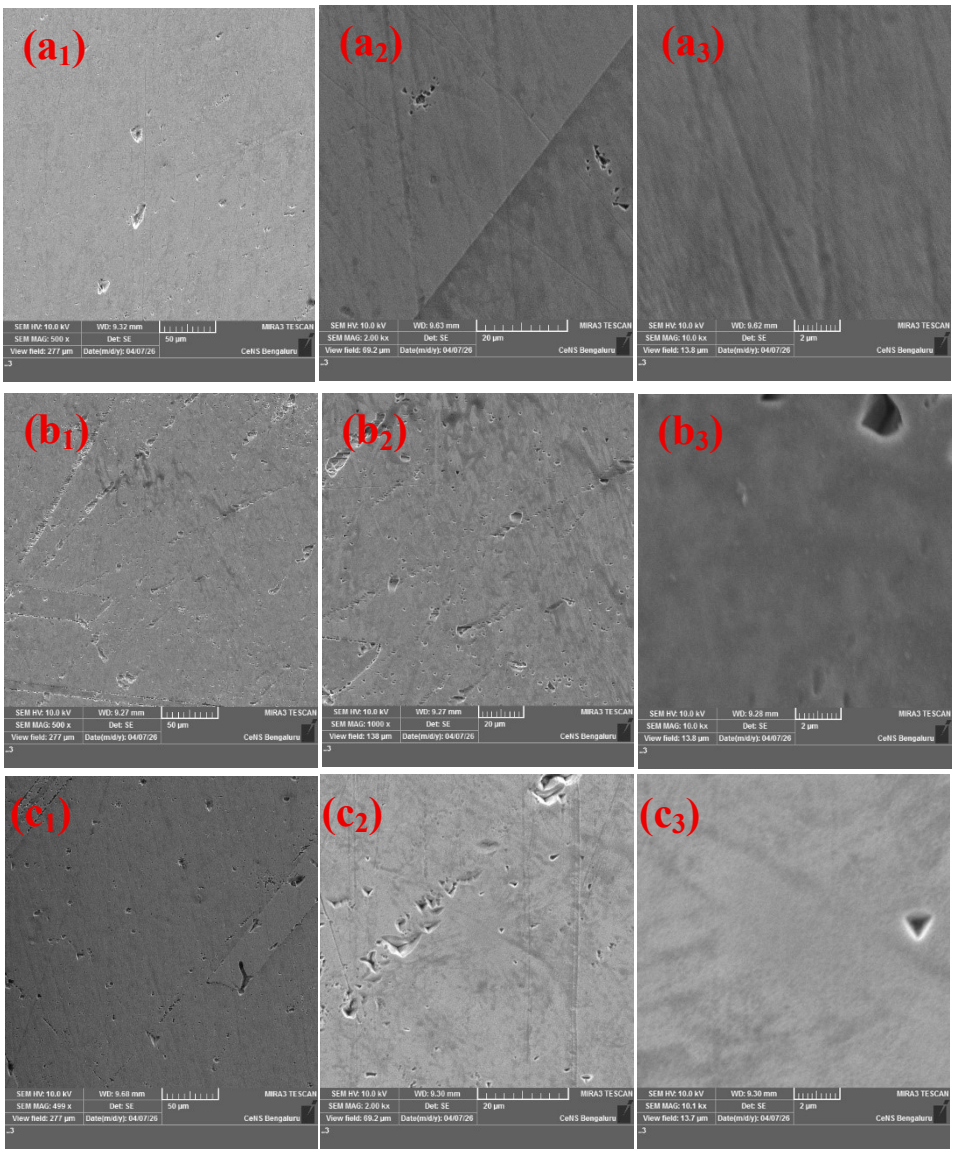
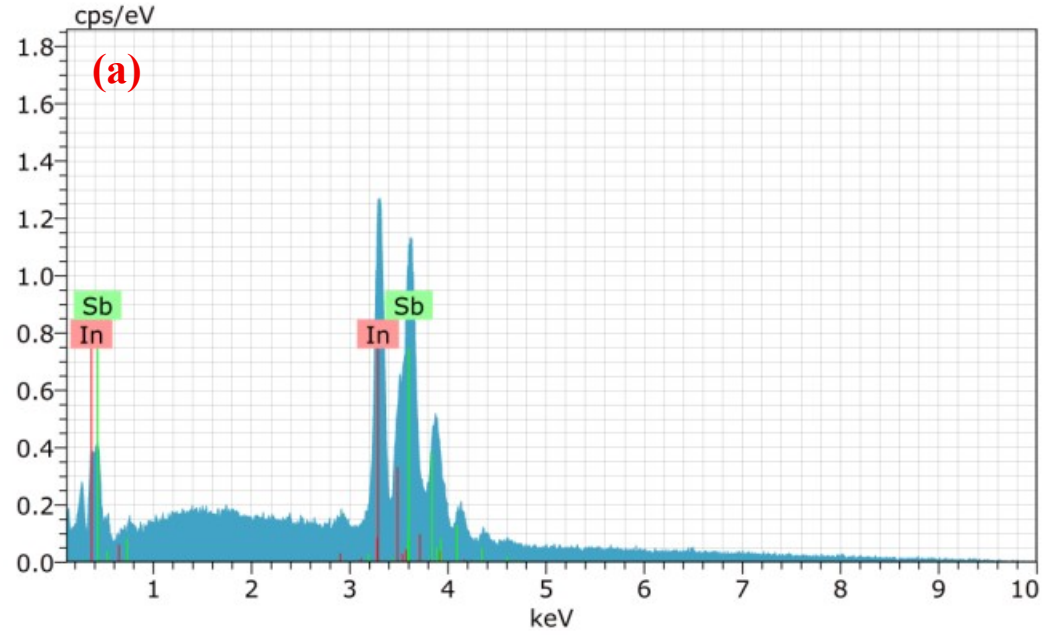
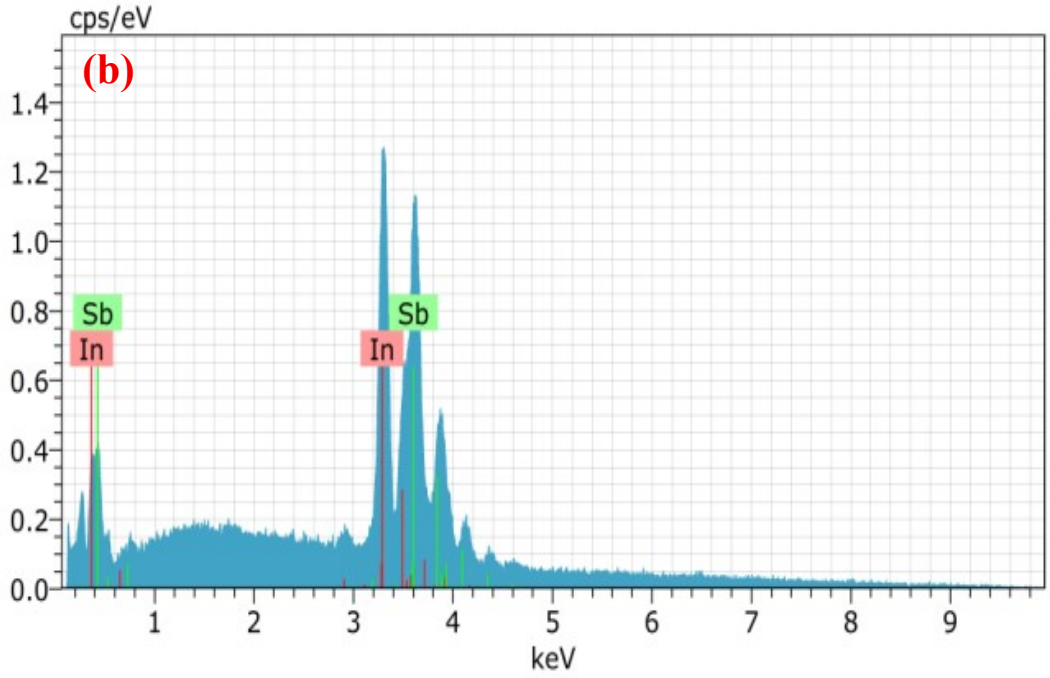


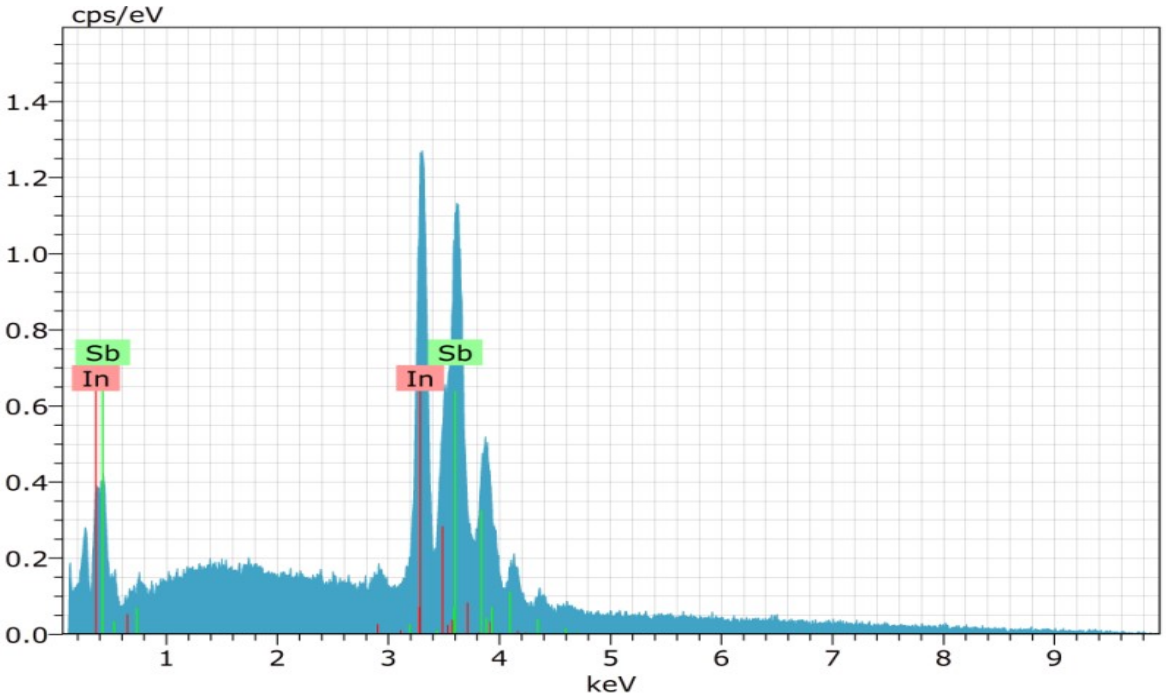
Fig. S1: FESEM pictures of SC InSb (a_1-a_3), AQ InSb (b_1-b_3), and IWQ InSb (c_1-c_3 polished ingots.

Fig. S2 shows the EDX analysis of SC InSb (a), AQ InSb (b), IWQ InSb (c), samples. From the EDX Spectrum the presence of In and Sb was confirmed the InSb samples. The low-level oxygen peaks related to surface oxidation of the samples. The reason for carbon peak was the double side carbon tape was used to load the samples. The elemental compositions of all the





samples are revealed in Table T1.



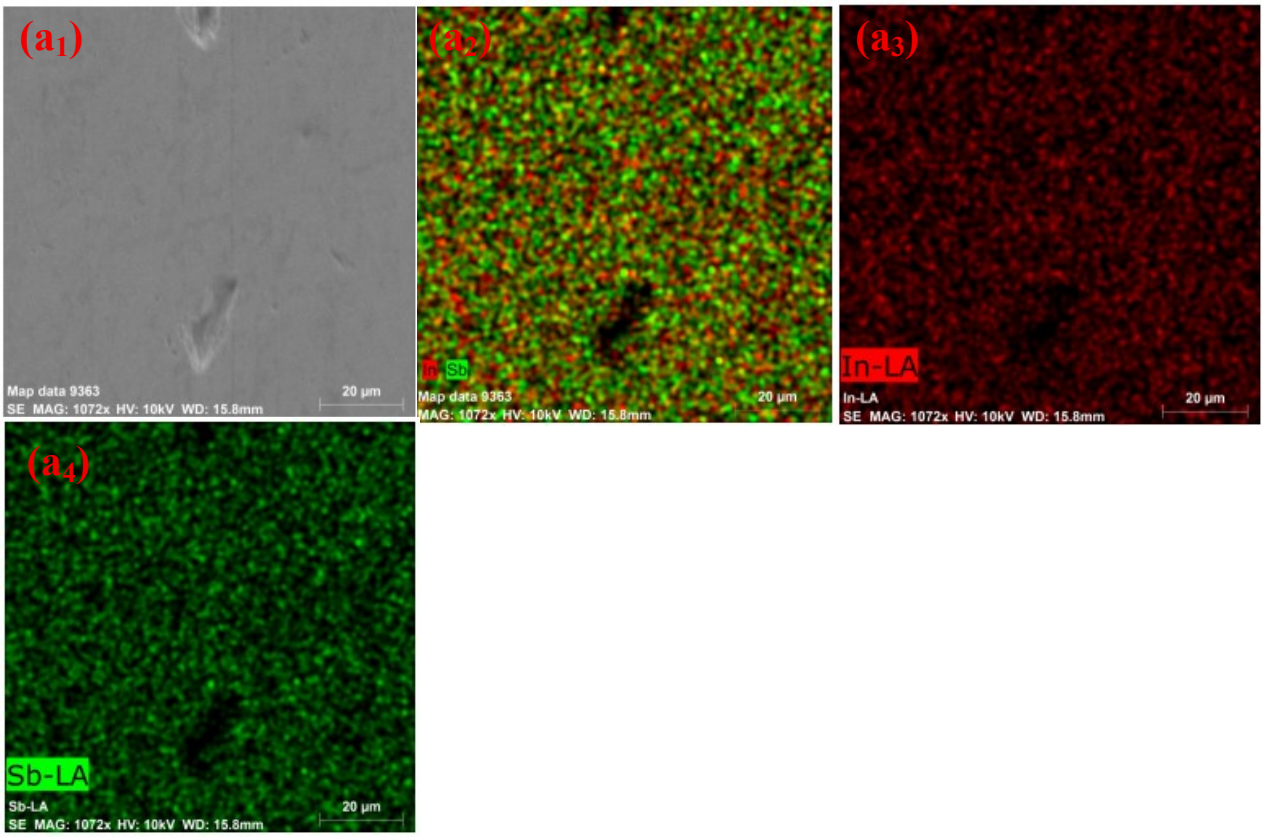
(c)

Fig. S2: EDX analysis of SC InSb (a), AQ InSb (b), IWQ InSb (c), samples.

Table T1: EDX - elemental compositional investigation of SC InSb (a), AQ InSb (b), IWQ InSb (c), samples.

Sample	Element	Weight %	Atomic %
SC InSb	In	46.29	47.75
	Sb	53.71	52.25
AQ InSb	In	46.19	47.55
	Sb	53.81	52.45
IWQ InSb	In	46.09	47.15
	Sb	53.91	52.85

Fig. S3 shows the FE-SEM basic elemental mapping analysis of the SC InSb (a_1-a_3), AQ InSb (b_1-b_3), and IWQ InSb (c_1-c_3) samples. The elemental mapping analysis validates the overall spreading of In and Sb elements in each InSb polycrystalline ingots.



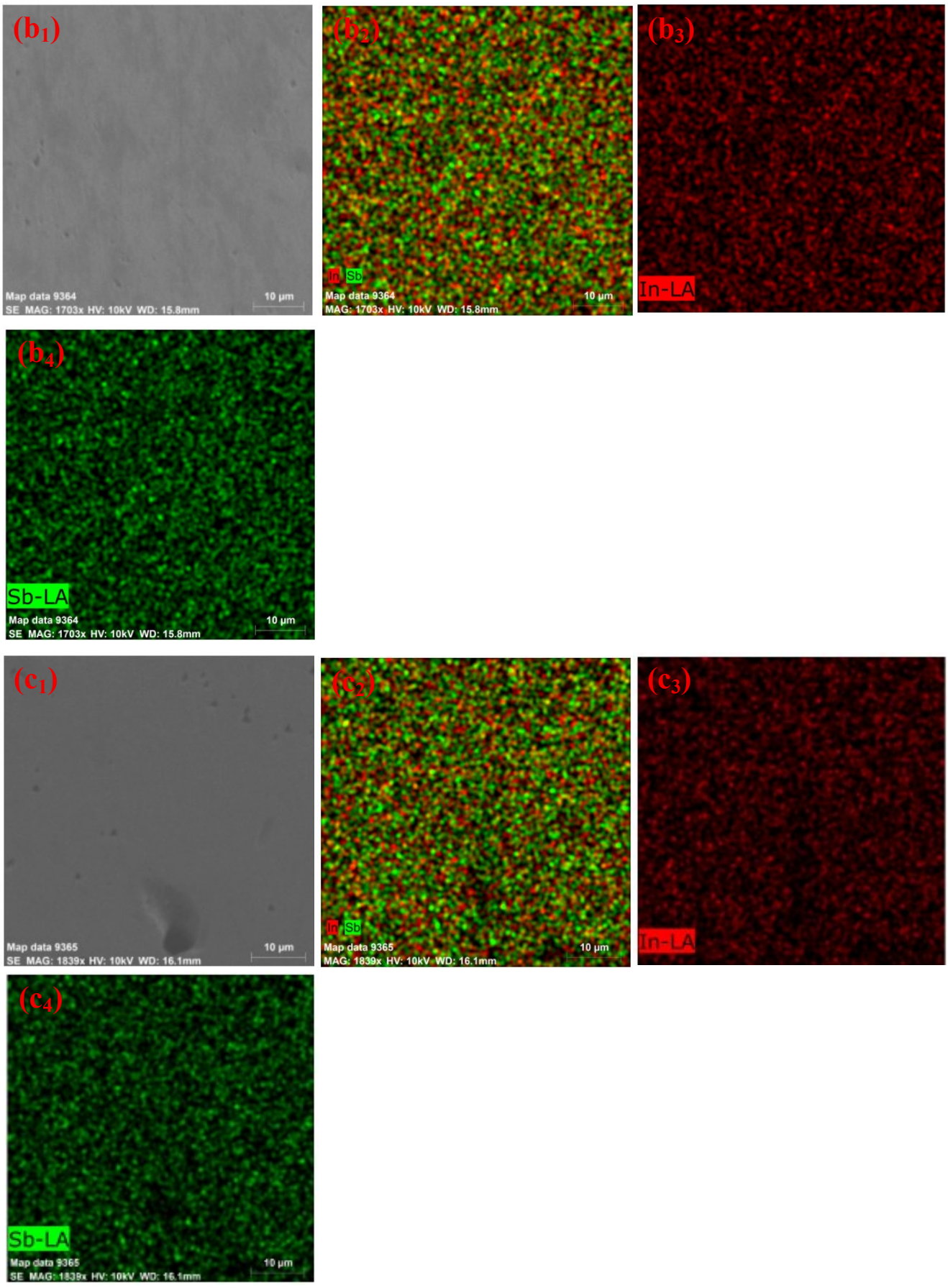


Fig. S3: FE-SEM elemental mapping analysis of the SC InSb (a_1-a_4) AQ InSb (b_1-b_4) and IWQ InSb (c_1-c_4).

Table S4 (a): grain boundary character distributions of SC InSb sample.

Sc InSb (Boundaries CSL)						
Parameters	**Centre portions**			**Edge portions**		
	∑3	**∑9**	**summary**	**∑3**	**∑9**	**summary**
Tolerance	8.66	5.00	-	8.66	5.00	-
Fraction	0.559	0.263	0.822	0.987	0.013	1.000
volume	0.0176	0.0102	0.0444	0.0176	0.0102	0.0444
MDF Value	31.81	25.91	18.51	56.19	1.28	22.53
Number	1589	748	-	836	11	-
Length	2.29 cm	1.07 cm	-	1.20 cm	158.77 microns	-
Lower angle (∑3, ∑9) grain boundaries						

Table S4 (b): grain boundary character distributions of AQ InSb sample.

AQ InSb (Boundaries CSL)											
Parameters	**Centre portions**					**Edge portions**					
	∑3	**∑9**	**∑27a**	**∑27b**	**summary**	**∑3**	**∑9**	**∑27a**	**∑27b**	**∑19a**	**summary**
Tolerance	**8.66**	**5.00**	**2.89**	**2.89**	**-**	8.66	5.00	2.89	2.89	3.44	-
Fraction	0.582	0.108	0.059	0.041	0.789	0.374	0.105	0.119	0.004	0.002	0.604
volume	0.0176	0.0102	0.0020	0.0039	0.0444	0.0176	0.0102	0.0020	0.0039	0.0022	0.0444
MDF Value	33.15	10.59	30.07	10.40	17.78	21.28	10.39	60.79	1.06	0.55	13.61
Number	2795	516	282	195	-	1630	460	518	18	8	-
Length	4.03 cm	7.44 mm	4.07 mm	2.81 mm	-	2.35 cm	6.63 mm	7.47 mm	259.80 microns	115.47 microns	-
Lower angle (∑3, ∑9) and Higher angle (∑27a, ∑27b, ∑19a) grain boundaries											

Table S4 (c): grain boundary character distributions of IWQ InSb sample.

IWQ InSb (Boundaries CSL)													
Parameters	**Centre portions**							**Edge portions**					
	∑3	**∑9**	**∑27a**	**∑27b**	**∑35b**	**∑19b**	**summary**	**∑3**	**∑9**	**∑27a**	**∑27b**	**∑19a**	**summary**
Tolerance	8.66	5.00	2.89	2.89	2.54	3.44	-	8.66	5.00	2.89	2.89	3.44	-
Fraction	0.531	0.077	0.038	0.019	0.005	0005	0.675	0.564	0.099	0.045	0.032	0.001	0.742
volume	0.0176	0.0102	0.0020	0.0039	0.0026	0.0022	0.0444	0.0176	0.0102	0.0020	0.0039	0.0033	0.0444
MDF Value	30.25	7.59	19.27	4.95	1.79	2.10	15.21	32.12	9.75	22.86	8.20	0.44	16.71
Number	5957	863	422	217	53	52	-	8932	1566	707	507	23	-
Length	8.59 cm	1.24 cm	6.09 mm	3.13 mm	764.98 mm	750.55 microns	-	12.89 cm	2.260 cm	1.02 cm	7.31 mm	331.97 microns	-
Lower angle (∑3, ∑9) and Higher angle (∑27a, ∑27b, ∑35b, ∑19b) grain boundaries													