Supplementary Information (SI) for Journal of Materials Chemistry C.

Supporting Information

The Experimental Phase Equilibria Studies of the Fe-Sb-As System

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S1 The industrial applications of the Fe-Sb-As system

Peterson and Twidwell [1] reported the removal of arsenic by roasting with pyrite from Sb-As containing lead bullion was reported. Filippou et al. [2] reported 6 wt.% Sb in enargite ($Cu_3As_{0.8}Sb_{0.2}S_4$), a key mineral in copper–gold deposits. They also reported high As-containing minerals can be separated into two types of feed (As-rich and As-lean but rich in precious metals) by adjusting pulp-potential [2].

In new pyrometallurgical technology, As- and Sb-rich feeds are treated to sulfidization roasting under reducing conditions, halogenation, and carbothermic reduction to form copper arsenide [2]. Nazari et al. [3] identified the presence of As with Sb in minerals like arsenopyrite, oliverite, which are undesirable during copper extraction. These are removed via volatilization to improve crude Cu and sulfuric acid production from released SO_2. They also reported that arsenic can be removed as ferric arsenate [3].

Nshimiyimana et al. [4] identified Fe-Sb-As-containing arsenopyrite $(Fe_{0.95}Co_{0.05})(As_{0.97}Sb_{0.01})S$ and freibergite $(Ag_{5.7}Cu_{4.6}Fe_{1.8})(Sb_{3.9}As_{0.2})S_{13}$ minerals. Majzlan et al. [5] reported As-Sb and Fe-Sb-As components in trombolite and tetrahedrite $(Cu,Fe, Zn)_{12}(Sb,As)_4S_{13}$, respectively. Jurkovic [6] observed Fe-Sb-As metals in different minerals, including As-Sb bearing goethite (α-FeOOH), As-bearing tripuhyite ($FeSbO_4$), senarmontite (Sb_2O_3), and cervantite (Sb_2O_4) in soils.

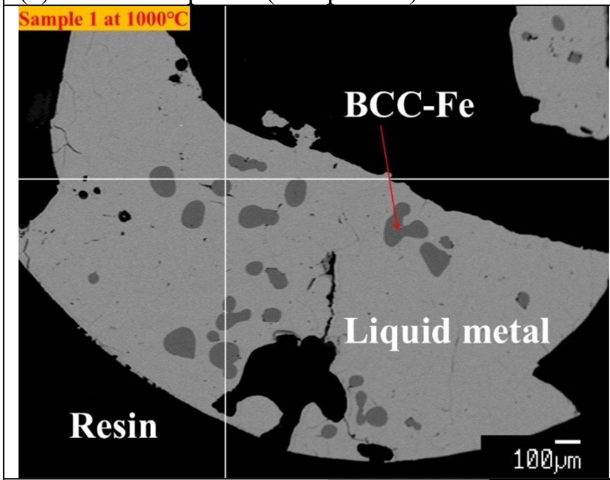
Zhang et al.[7] noted that Fe-Sb-As metals in acid mine drainage, caused by minerals exploration and utilization, rigorously contaminate ecological environments. They also reported that As-containing slag poses ecological risks, which can be mitigated by forming stable As phases during pyrometallurgical operations [8]. During Sn smelting, the slag contained around 10-15 wt.% Sb and 1-3 wt.% As. As-Sb dust contains 0.5–1% As and 2–4% Sb.

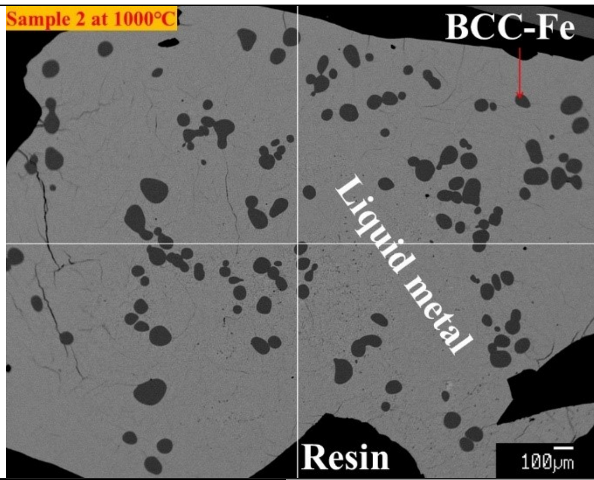
S2. The Fe-As system

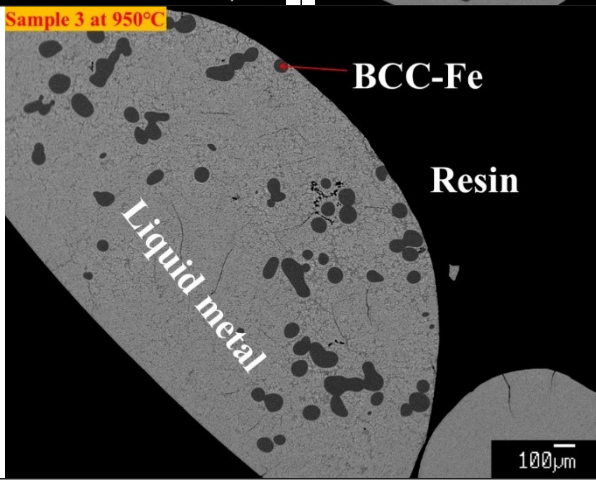
Friedrich [9] used thermal analysis and microscopy and determine the phase diagram from the compositions of 6-49 at. % As. Oberhoffer and Gallaschik [10] used thermal analysis, microscopy, and magnetic content analysis to determination the phase diagram from 0-32 at. % As and magnetic transition. Jones [11] measured diffusion of arsenic in iron and determine the saturation composition of iron (FCC) at 1423 K. Svechnikov and Gridnev [12] used a dilatometry, microscopy, and XRD to determine limits of the iron (FCC) saturation loop. Sawamura and Mori [13] used thermal analysis and microscopy and reported the solubility of arsenic in iron (FCC) based on extrapolations from measurements made on alloys of iron and arsenic containing low concentrations of carbon. Sawamura et al.[14] used a DTA to determine the phase diagram between 40 to 57 at. % As. Svechnikov and Shurin [15] used thermal analysis, microscopy, and XRD to determine the limits of the solubility of arsenic in iron (FCC). Svechnikov et al. [16] used microhardness, microscopy, and XRD to determine the solid solubility of arsenic in iron (BCC). Clark [17] used DTA, optical microscopy and XRD to study the Fe-As system. Clark [18] used optical microscopy and XRD to study the Fe-As system. Predel and Frebel [19] used DTA to determine the solid solubility of arsenic in iron (BCC). Bozic [20] used thermal analysis to determine the maximum solid solubility of arsenic in iron (BCC) at the eutectic temperature. Pei et al. [21] and Kidari and Chartrand [22] thermodynamically assessed the

Fe-As system. Ugai et al. [23] used DTA and XRD and reported the pressure-temperature-composition diagram for the Fe-As system for 0.50-1.0 at. % As.

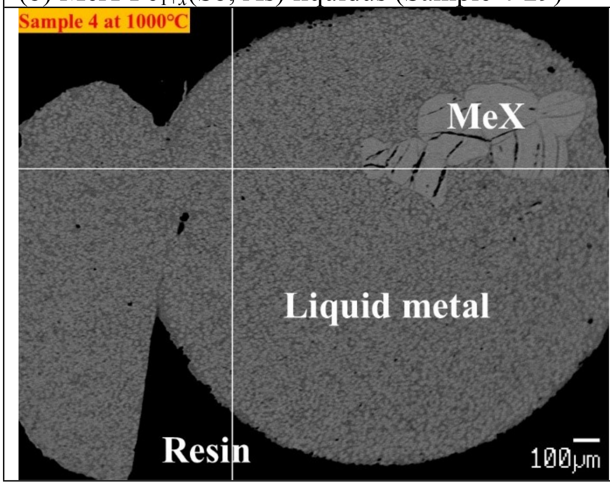
(a) BCC-Fe liquidus (Sample 1-3)

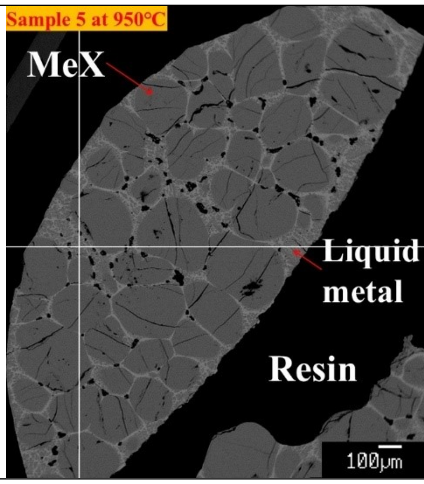


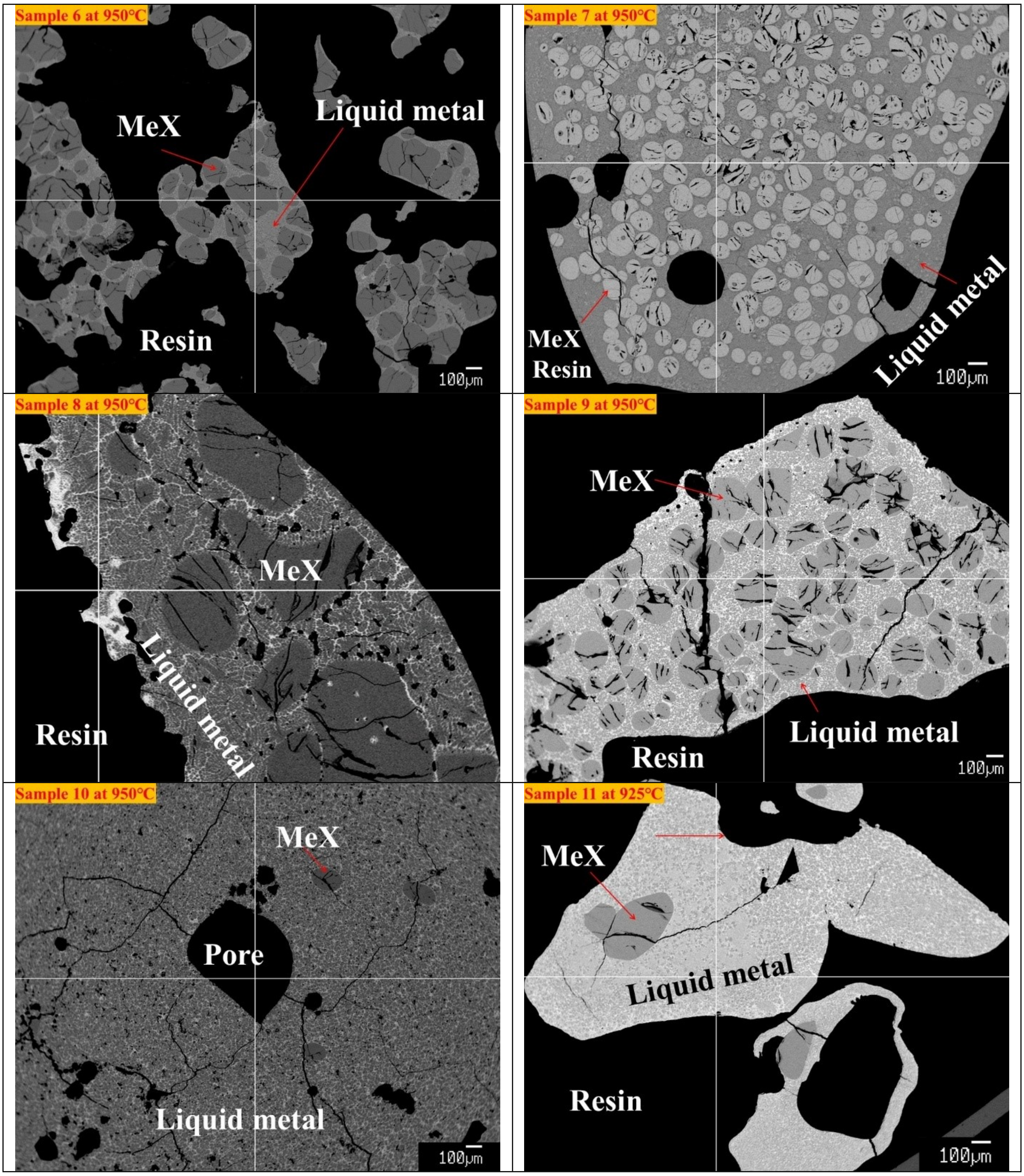


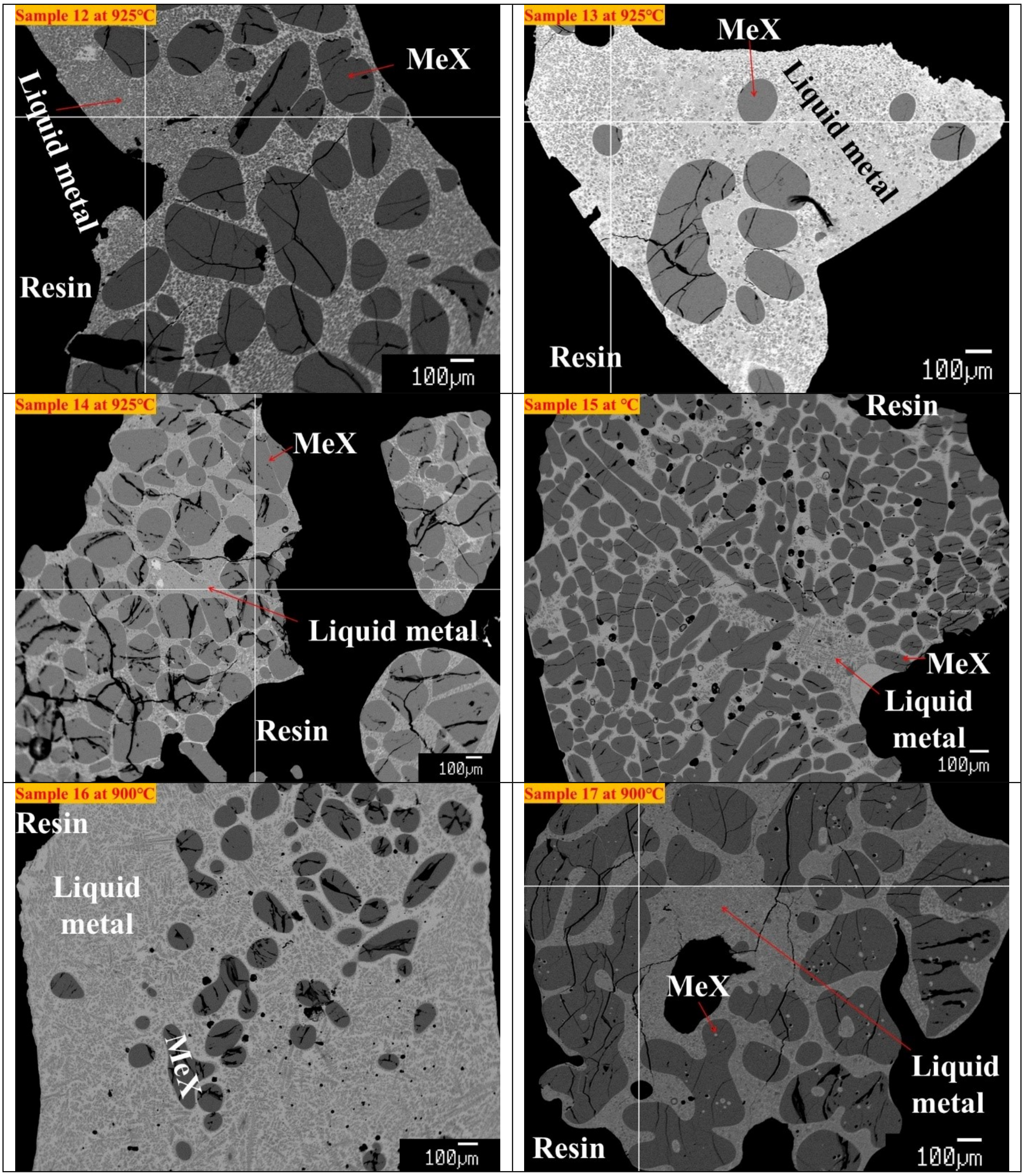


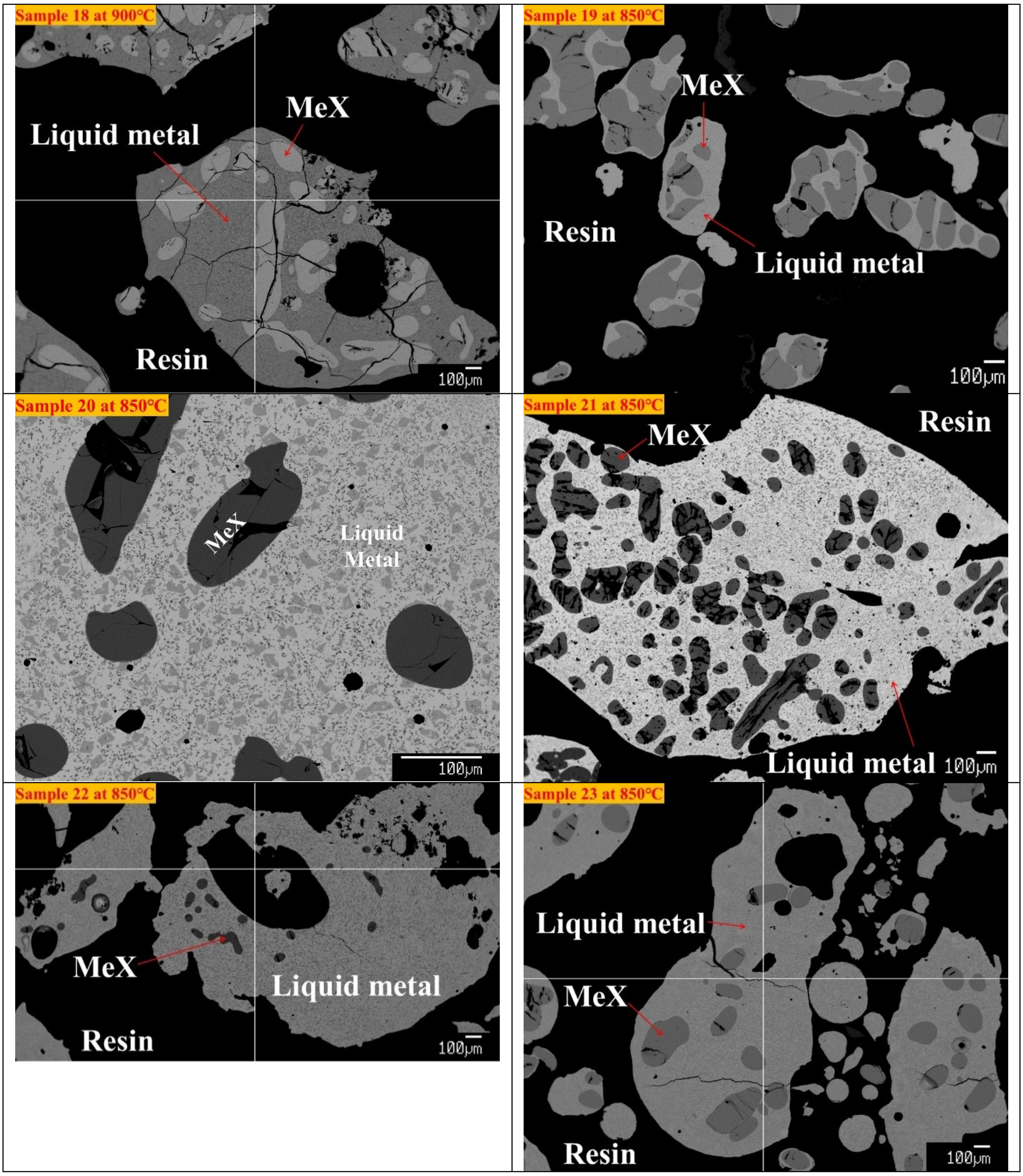
(b) MeX-Fe$_{1+x}$(Sb, As) liquidus (Sample 4-29)

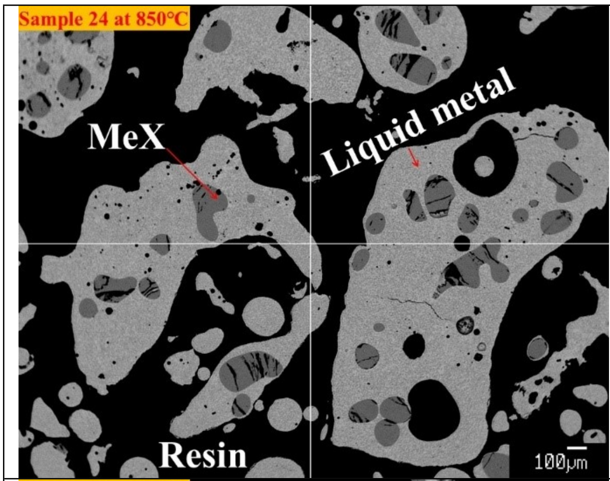


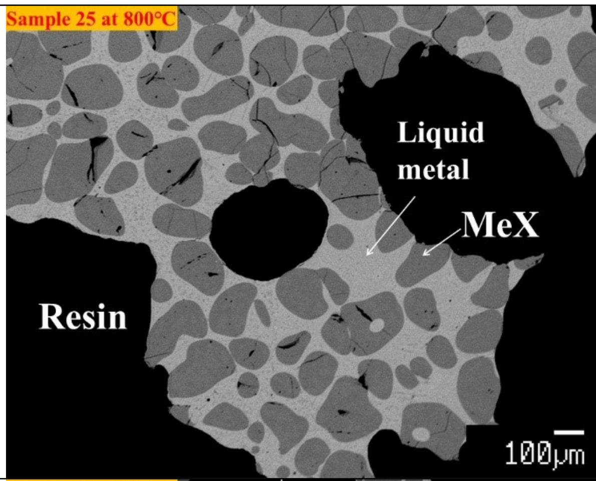


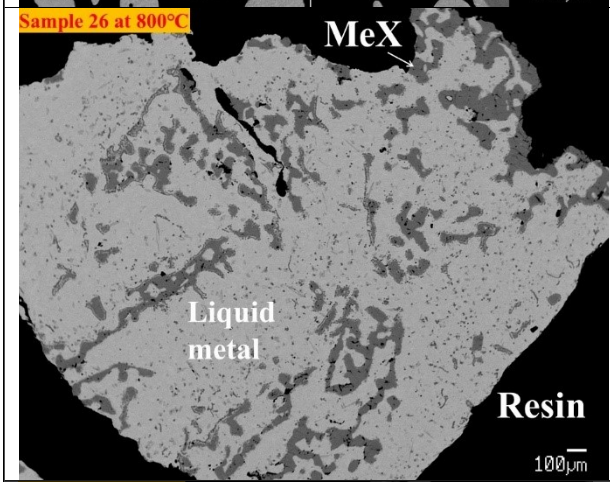

Sample 6 at 950°C
MeX
Liquid metal
Resin
100μm
Sample 7 at 950°C
MeX
Resin
Liquid metal
100μm
Sample 8 at 950°C
MeX
Liquid metal
Resin
Sample 9 at 950°C
MeX
Liquid metal
Resin
100μm
Sample 10 at 950°C
MeX
Pore
Liquid metal
100μm
Sample 11 at 925°C
MeX
Liquid metal
Resin
100μm

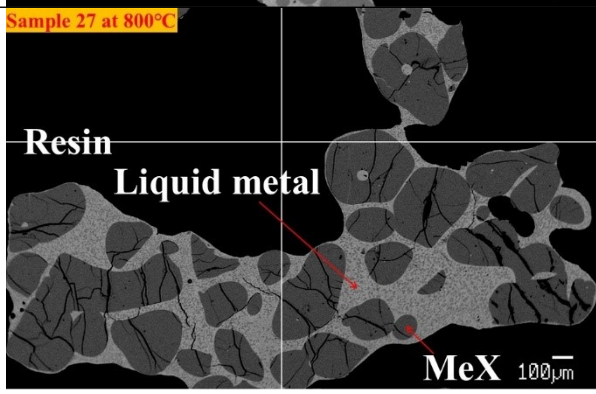

Sample 12 at 925°C
MeX
Liquid metal
Resin
100μm
Sample 13 at 925°C
MeX
Liquid metal
Resin
100μm
Sample 14 at 925°C
MeX
Liquid metal
Resin
100μm
Sample 15 at °C
Resin
MeX
Liquid metal
100μm
Sample 16 at 900°C
Resin
Liquid metal
MeX
100μm
Sample 17 at 900°C
MeX
Liquid metal
Resin
100μm

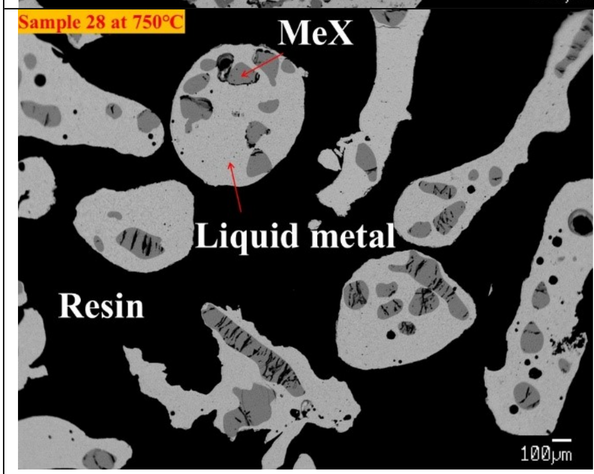

Sample 18 at 900°C
Liquid metal
MeX
Resin
100μm
Sample 19 at 850°C
MeX
Resin
Liquid metal
100μm
Sample 20 at 850°C
MeX
Liquid
Metal
100μm
Sample 21 at 850°C
MeX
Resin
Liquid metal
100μm
Sample 22 at 850°C
MeX
Liquid metal
Resin
100μm
Sample 23 at 850°C
Liquid metal
MeX
Resin
100μm

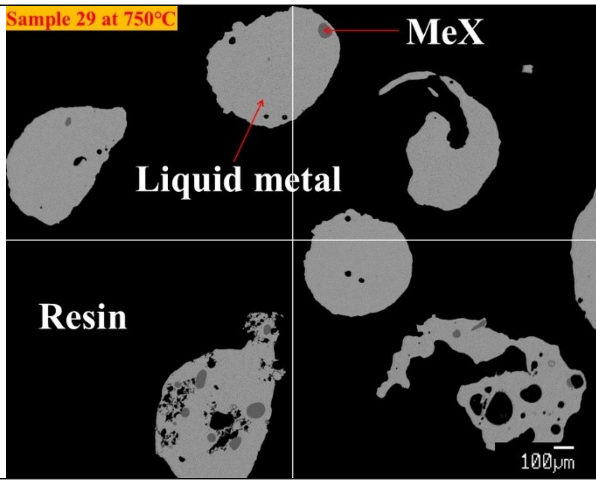




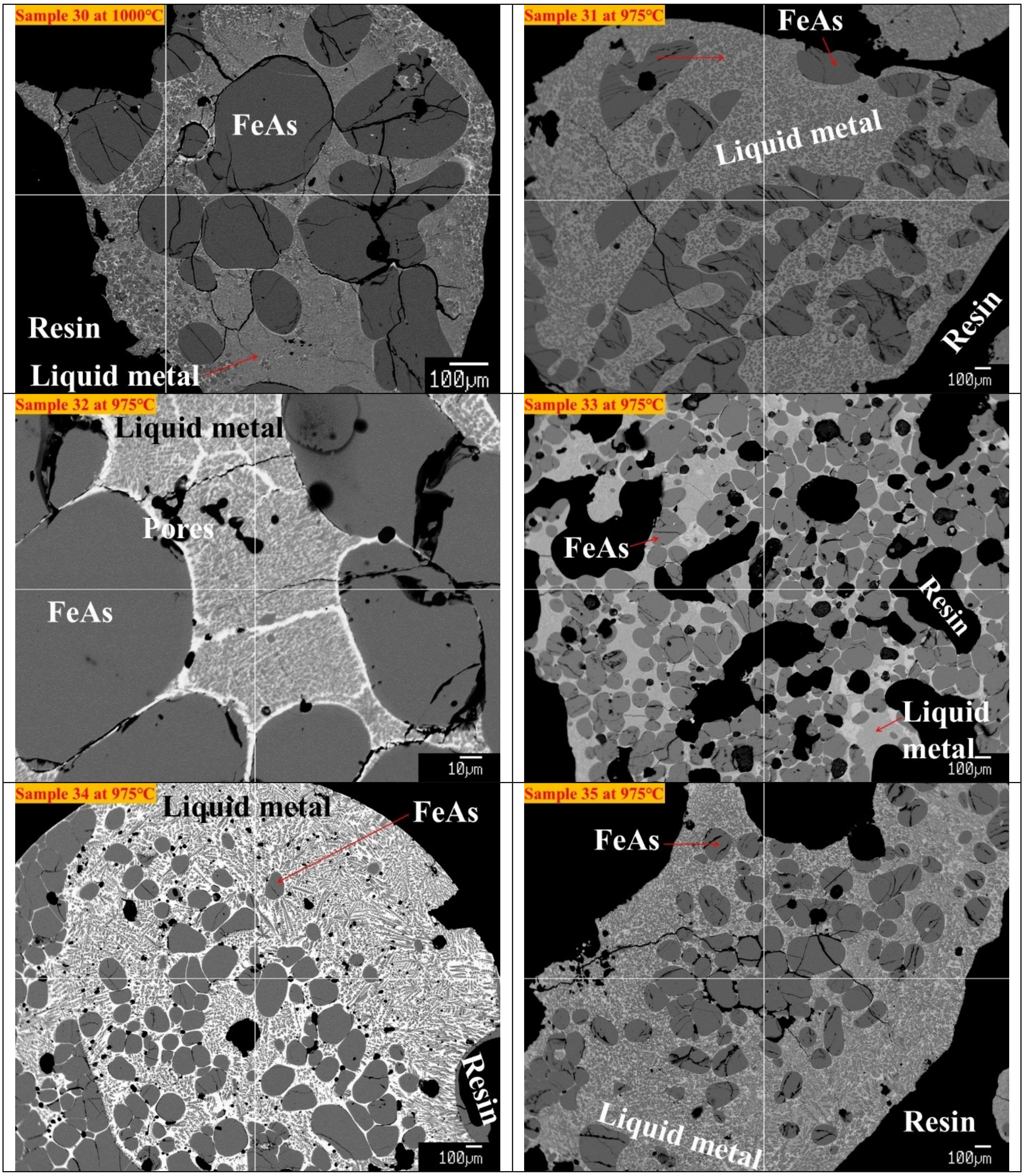


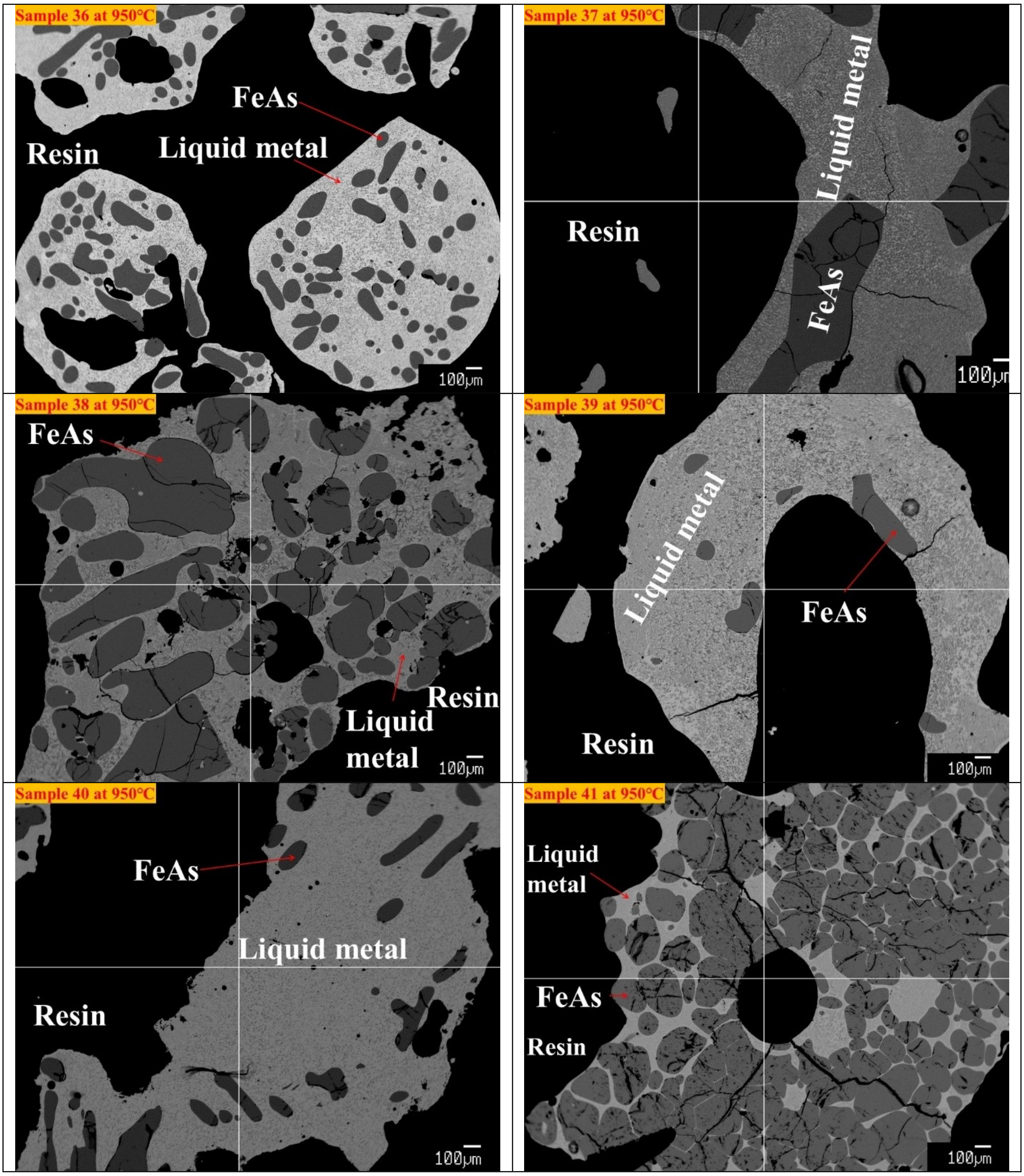


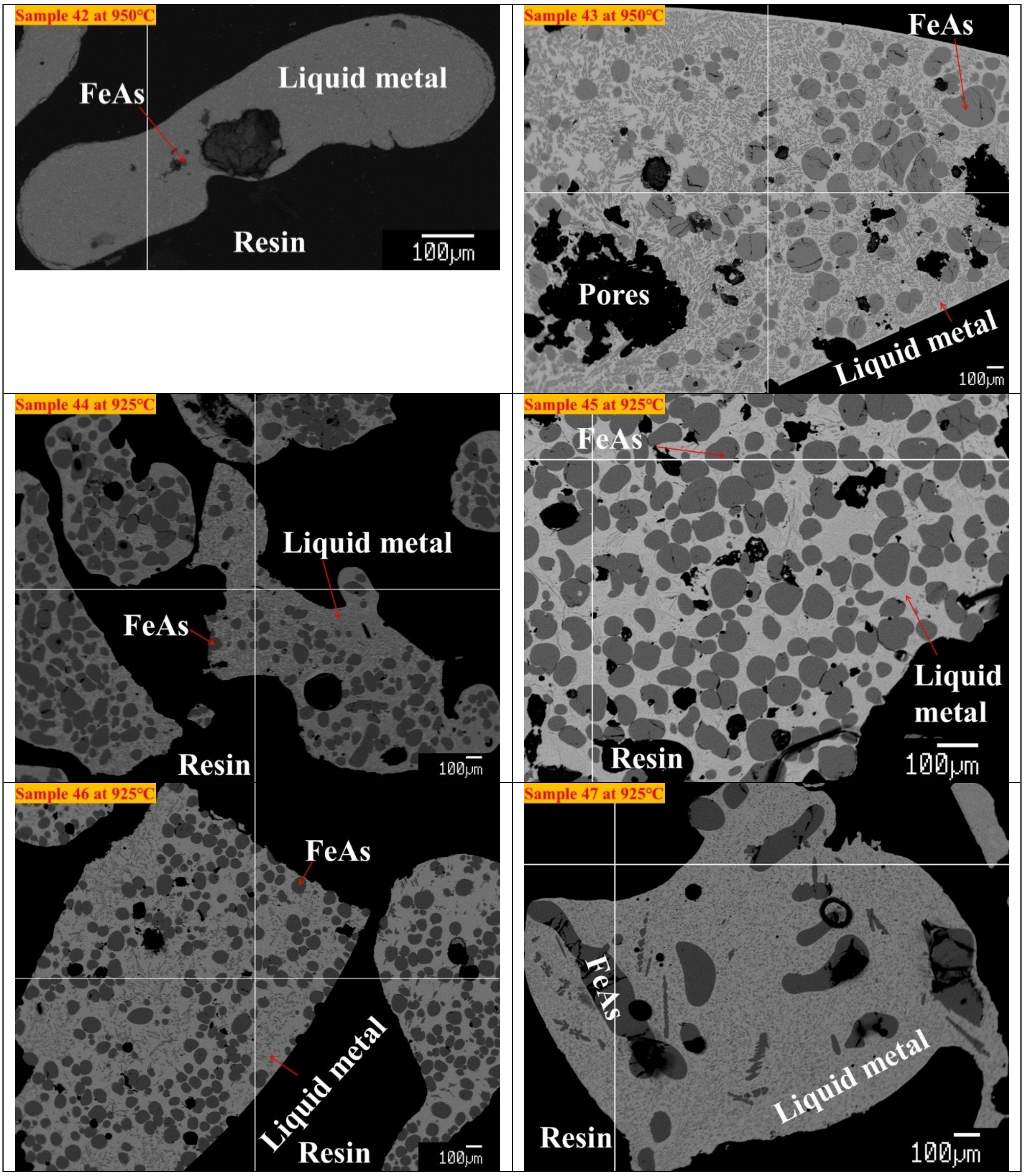


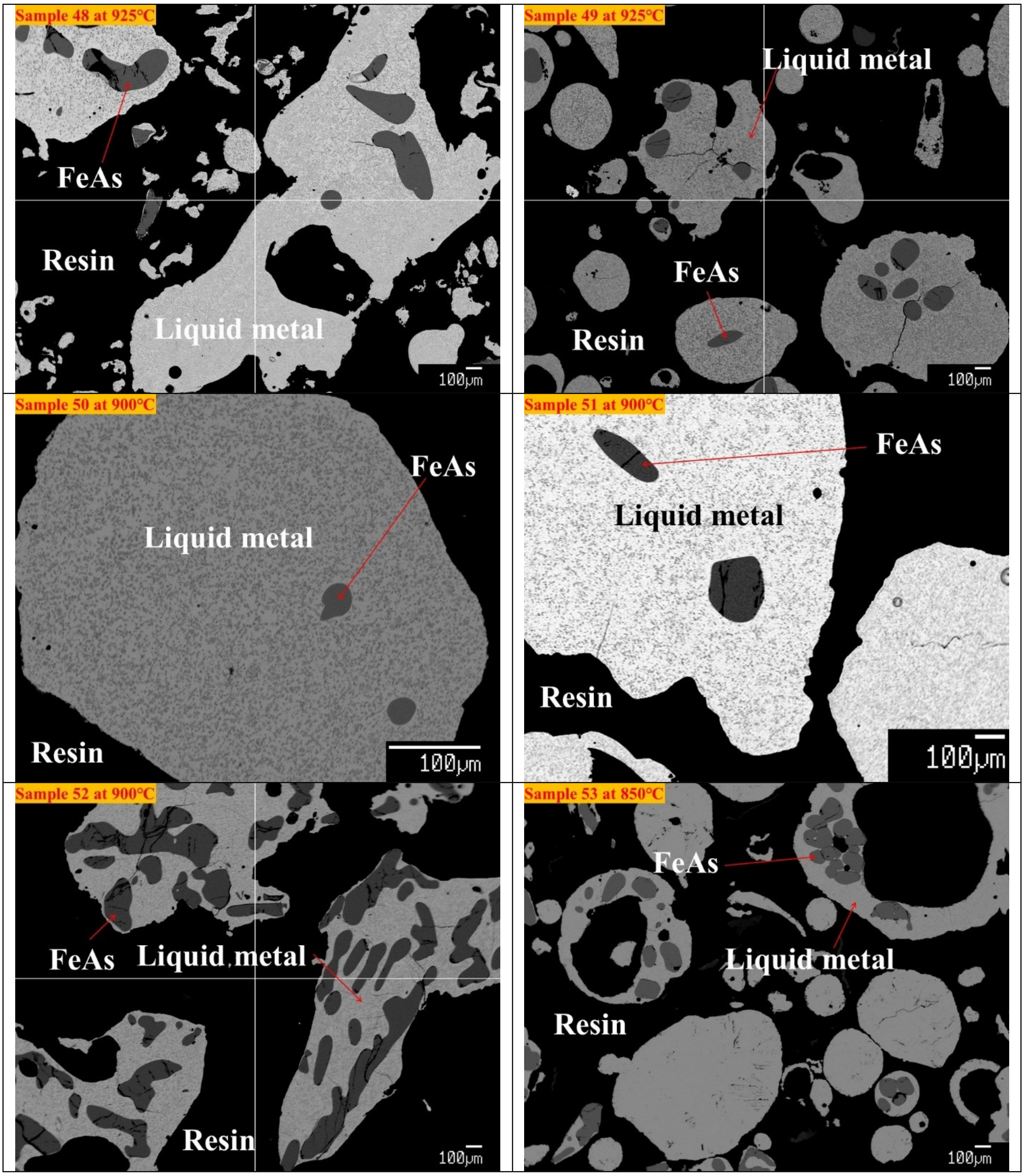


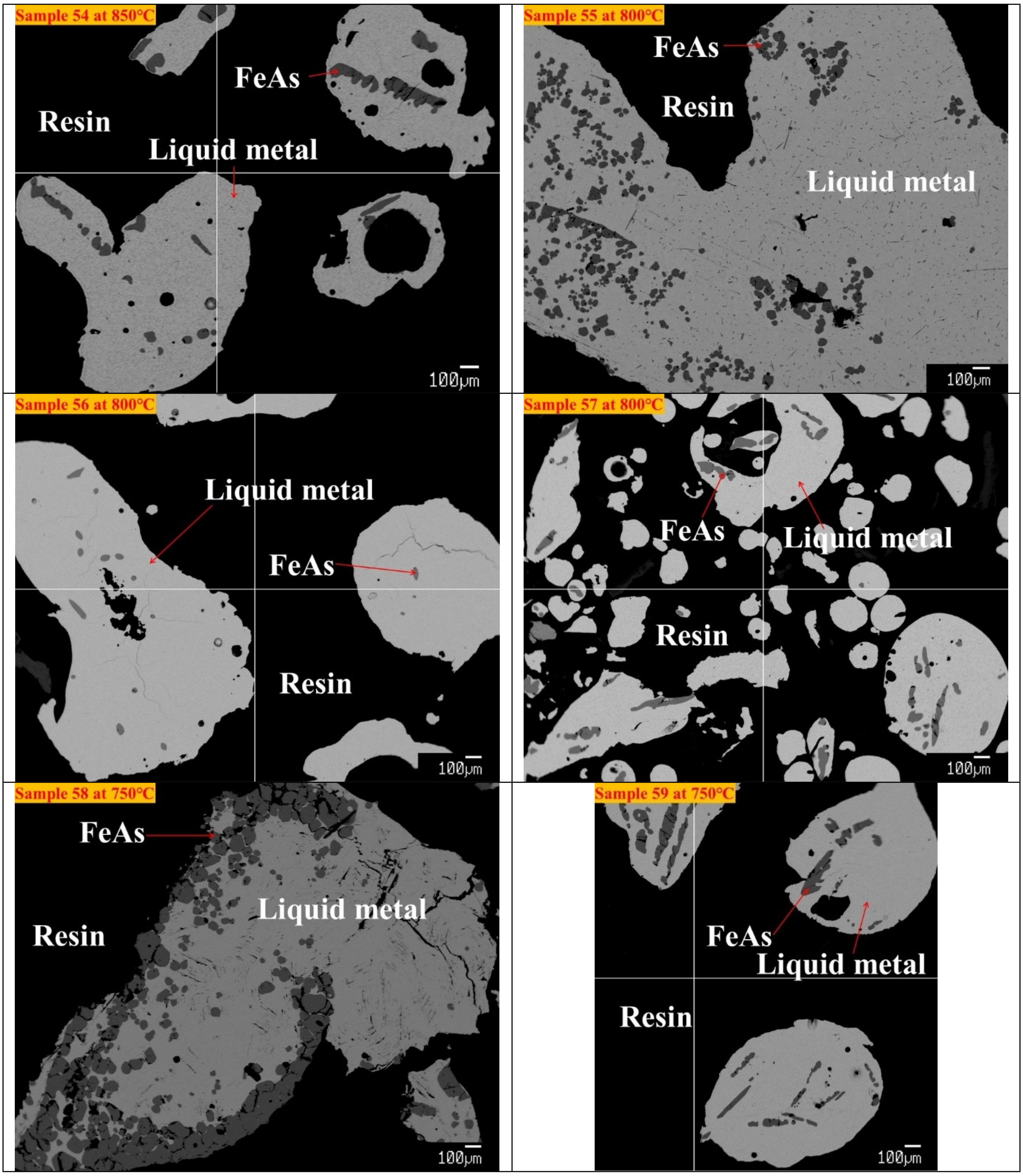
(c) Fe(As, Sb) liquidus (Sample 30-61)

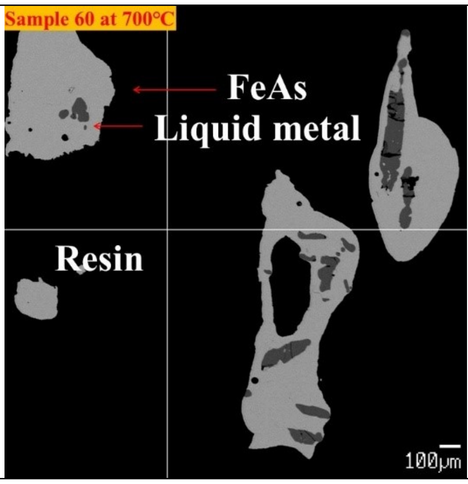

Sample 30 at 1000°C
FeAs
Resin
Liquid metal
100μm
Sample 31 at 975°C
FeAs
Liquid metal
Resin
100μm
Sample 32 at 975°C
Liquid metal
Pores
FeAs
10μm
Sample 33 at 975°C
FeAs
Resin
Liquid metal
100μm
Sample 34 at 975°C
Liquid metal
FeAs
Resin
100μm
Sample 35 at 975°C
FeAs
Resin
Liquid metal
100μm

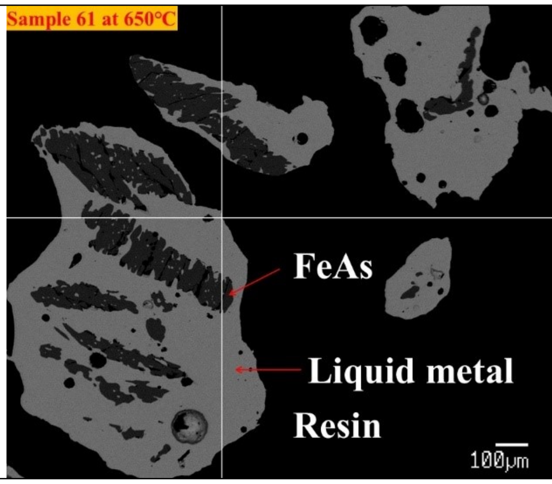

Sample 36 at 950°C
FeAs
Liquid metal
Resin
100μm
Sample 37 at 950°C
Liquid metal
Resin
FeAs
Sample 38 at 950°C
FeAs
Resin
Liquid
metal
100μm
Sample 39 at 950°C
Liquid metal
FeAs
Resin
100μm
Sample 40 at 950°C
FeAs
Liquid metal
Resin
100μm
Sample 41 at 950°C
Liquid
metal
FeAs
Resin
100μm


Sample 42 at 950°C
FeAs
Liquid metal
Resin
100μm
Sample 43 at 950°C
FeAs
Pores
Liquid metal
100μm
Sample 44 at 925°C
Liquid metal
FeAs
Resin
100μm
Sample 45 at 925°C
FeAs
Liquid metal
Resin
100μm
Sample 46 at 925°C
FeAs
Liquid metal
Resin
100μm
Sample 47 at 925°C
FeAs
Liquid metal
Resin
100μm

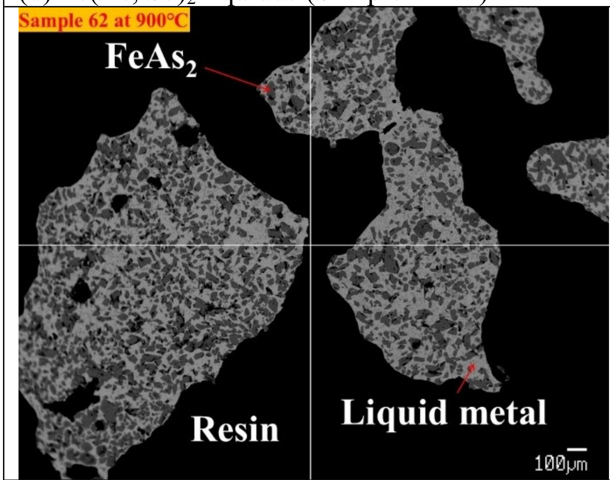

Sample 48 at 925°C
FeAs
Resin
Liquid metal
100μm
Sample 49 at 925°C
Liquid metal
FeAs
Resin
100μm
Sample 50 at 900°C
FeAs
Liquid metal
Resin
100μm
Sample 51 at 900°C
FeAs
Liquid metal
Resin
100μm
Sample 52 at 900°C
FeAs
Liquid metal
Resin
100μm
Sample 53 at 850°C
FeAs
Liquid metal
Resin
100μm

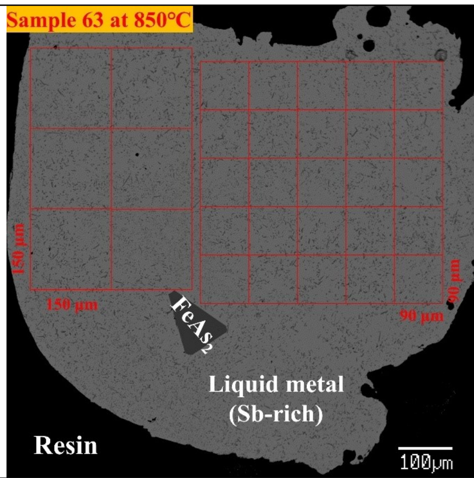

Sample 54 at 850°C
FeAs
Resin
Liquid metal
100μm
Sample 55 at 800°C
FeAs
Resin
Liquid metal
100μm
Sample 56 at 800°C
Liquid metal
FeAs
Resin
100μm
Sample 57 at 800°C
FeAs
Liquid metal
Resin
100μm
Sample 58 at 750°C
FeAs
Liquid metal
Resin
100μm
Sample 59 at 750°C
FeAs
Liquid metal
Resin
100μm

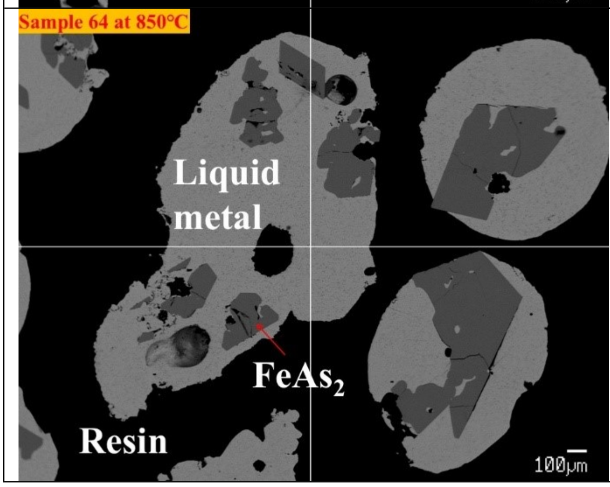


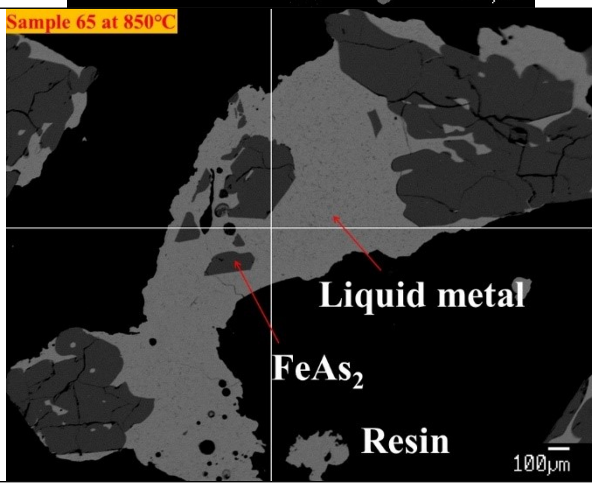


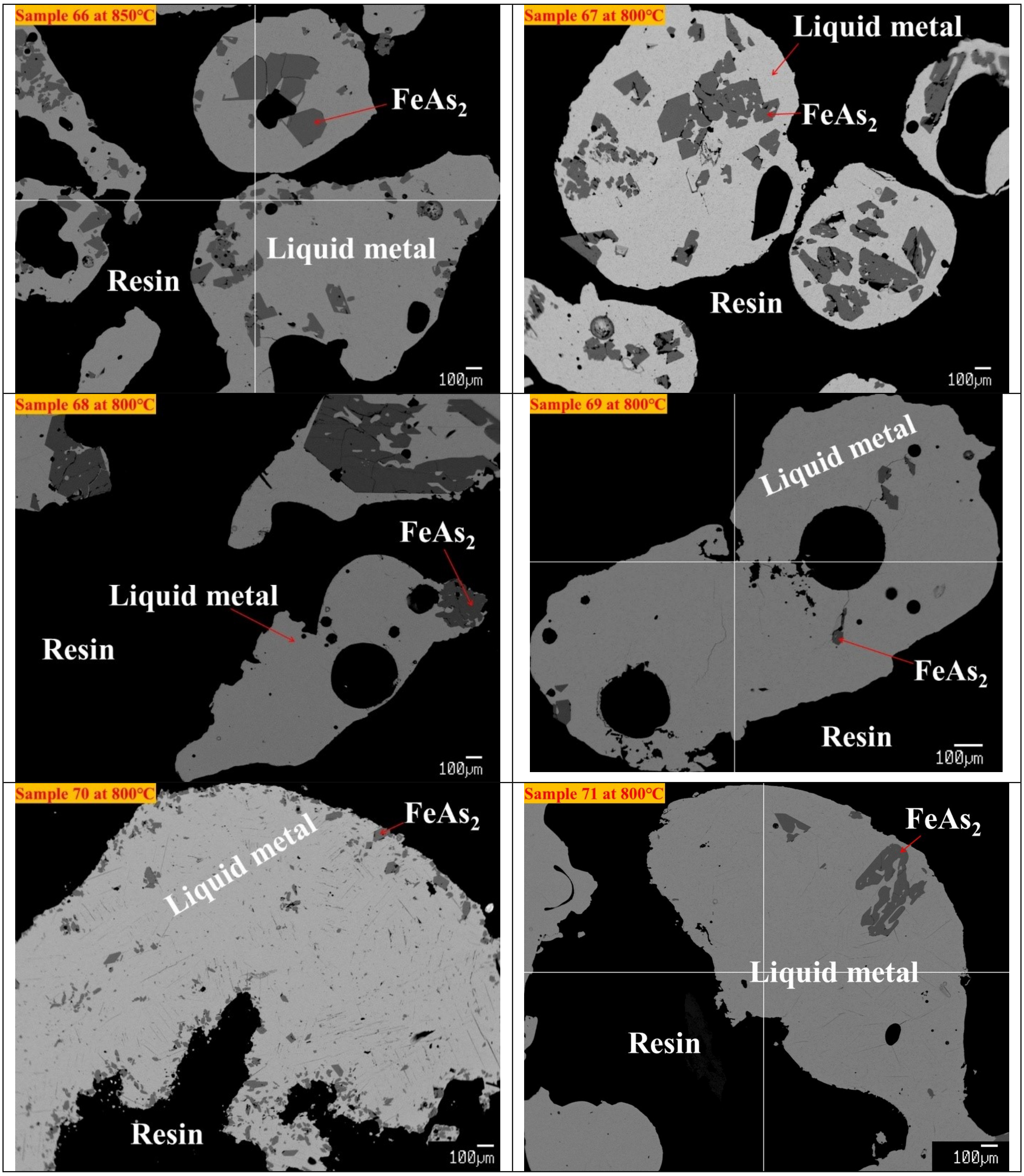
(d) $Fe(As, Sb)_2$ liquidus (Sample 62-80)



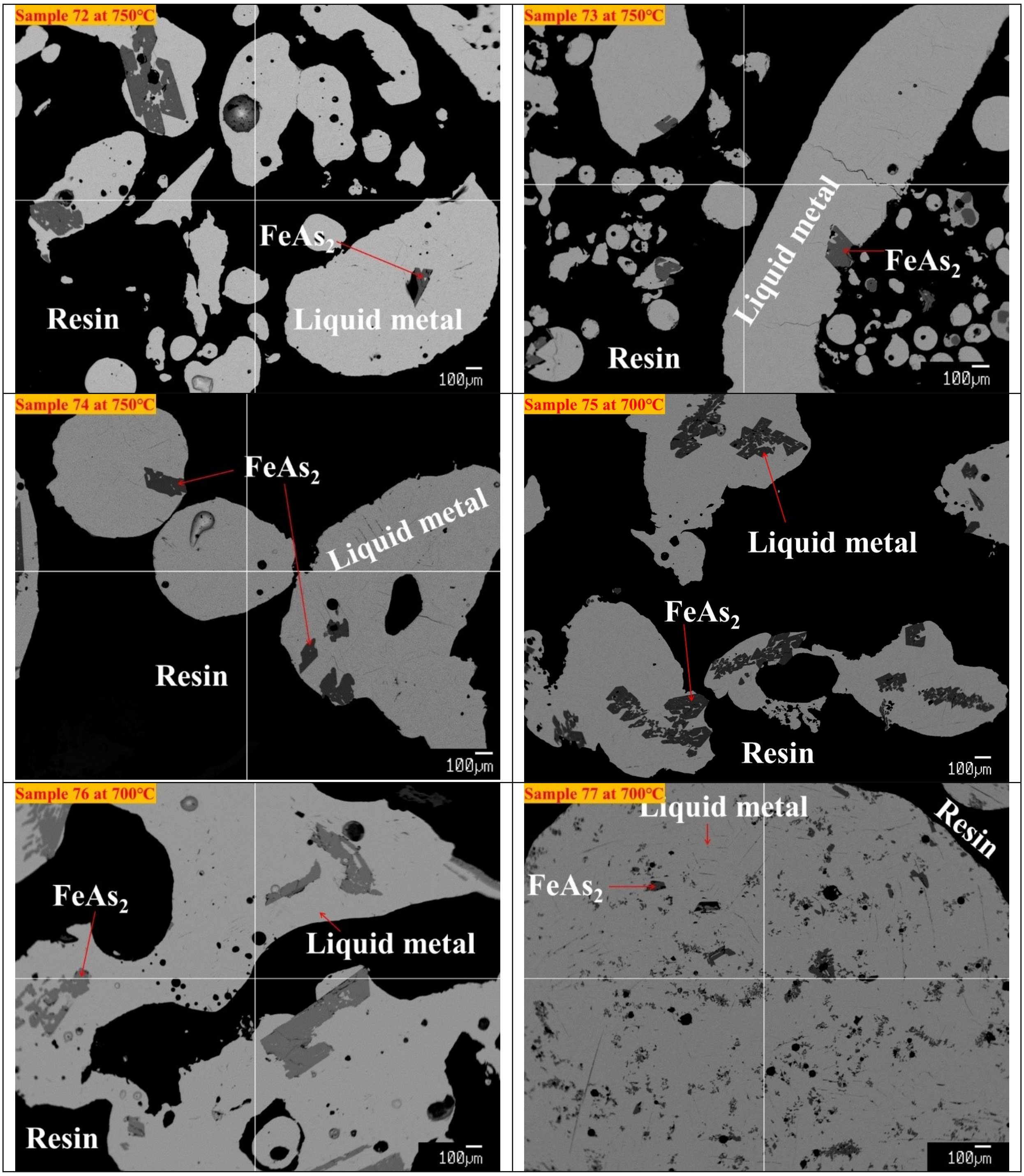




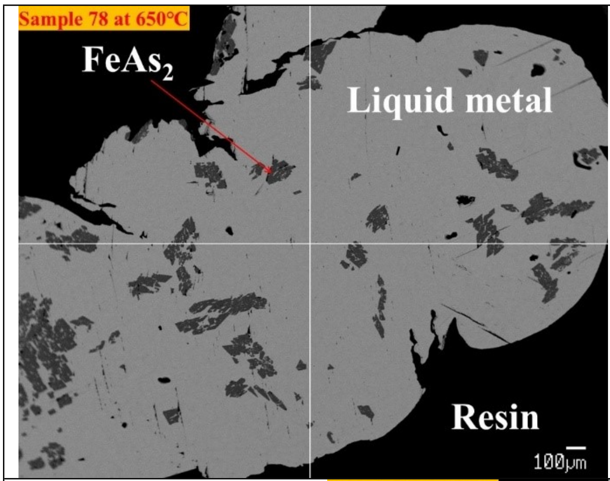


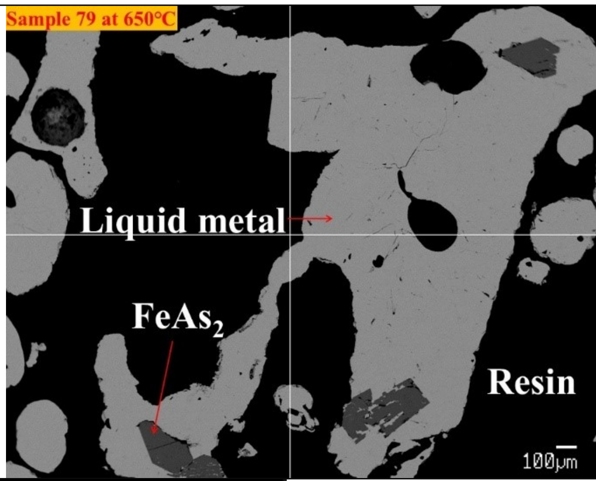


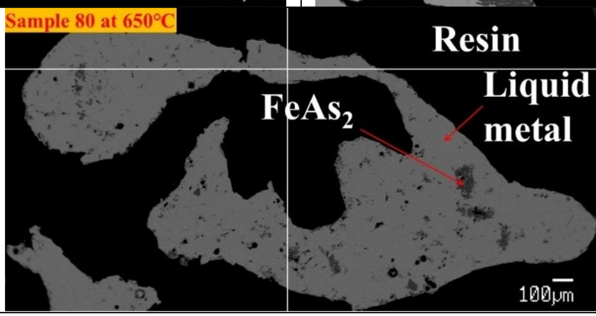
Sample 66 at 850°C
FeAs2
Liquid metal
Resin
100μm
Sample 67 at 800°C
Liquid metal
FeAs2
Resin
100μm
Sample 68 at 800°C
FeAs2
Liquid metal
Resin
100μm
Sample 69 at 800°C
Liquid metal
FeAs2
Resin
100μm
Sample 70 at 800°C
FeAs2
Liquid metal
Resin
100μm
Sample 71 at 800°C
FeAs2
Liquid metal
Resin
100μm



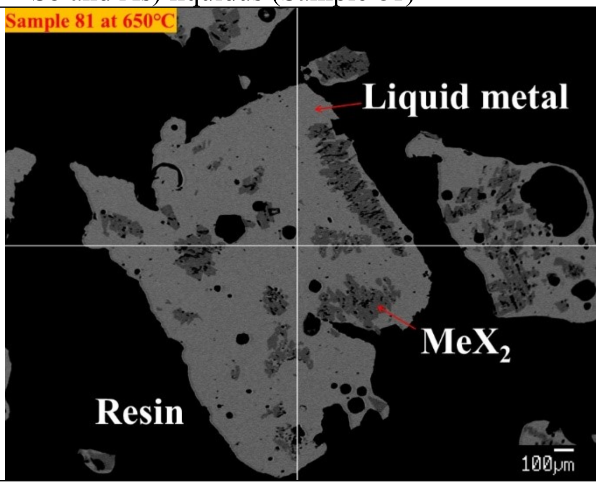
Sample 72 at 750°C
FeAs2
Resin
Liquid metal
100μm
Sample 73 at 750°C
Liquid metal
FeAs2
Resin
100μm
Sample 74 at 750°C
FeAs2
Liquid metal
Resin
100μm
Sample 75 at 700°C
Liquid metal
FeAs2
Resin
100μm
Sample 76 at 700°C
FeAs2
Liquid metal
Resin
100μm
Sample 77 at 700°C
Liquid metal
Resin
FeAs2
100μm



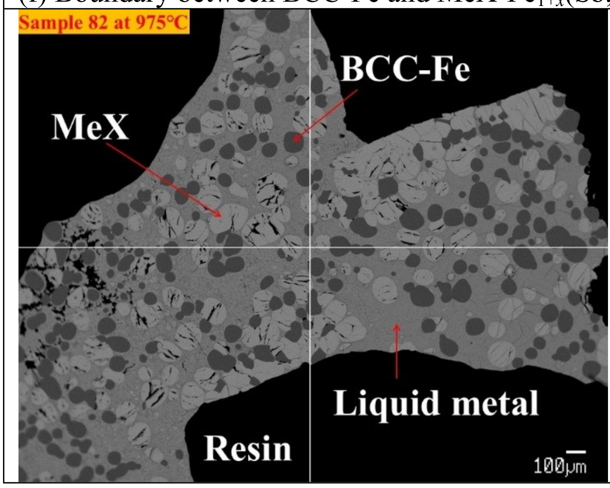


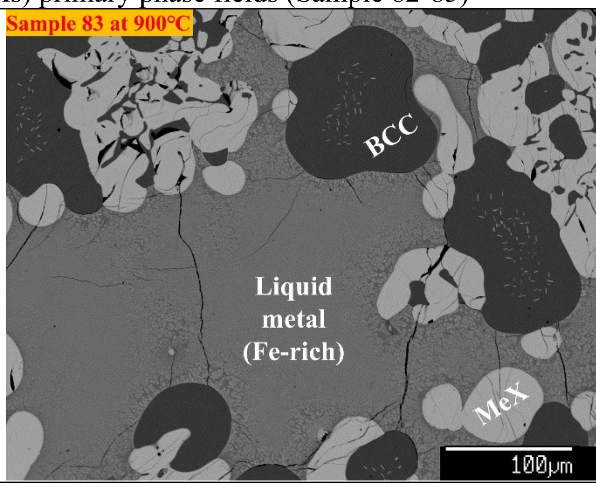


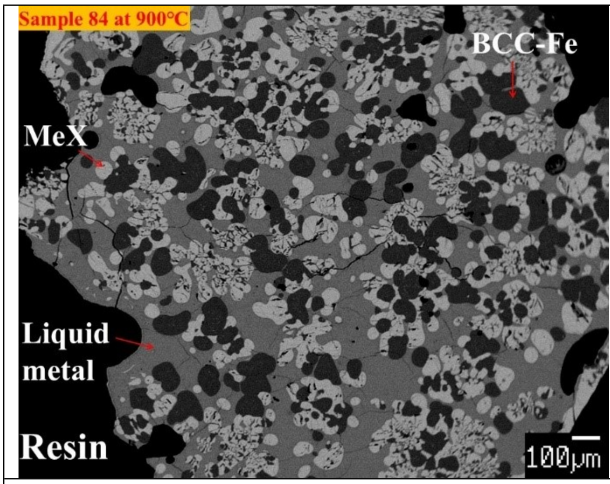
(e) MeX_2 (Me = Fe and X = Sb and As) liquidus (Sample 81)

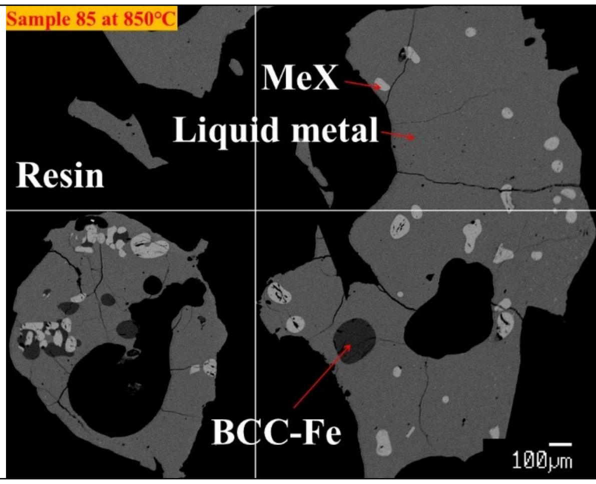


(f) Boundary between BCC-Fe and MeX-Fe_{1+x}(Sb, As) primary phase fields (Sample 82-85)

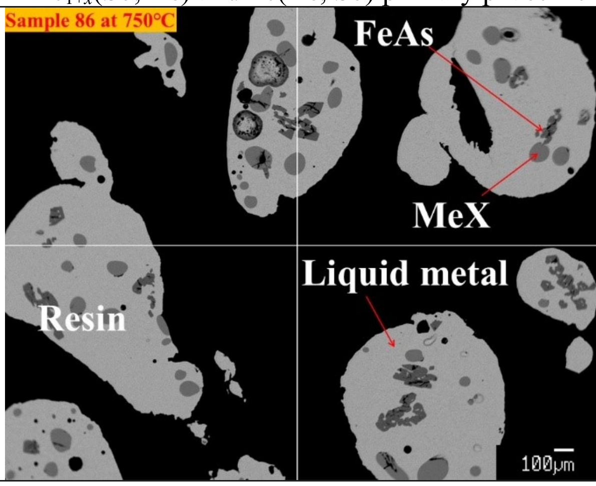




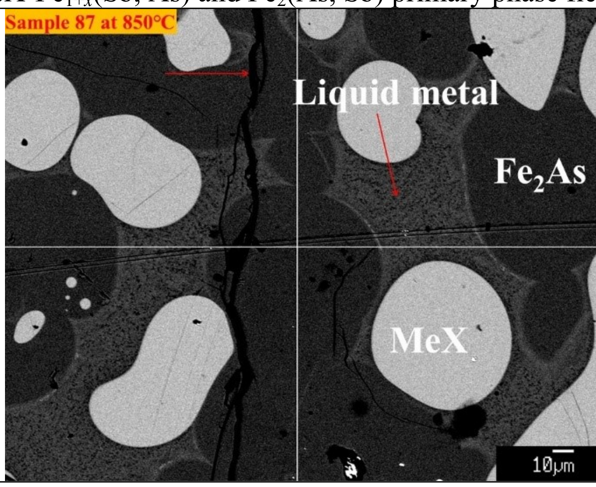




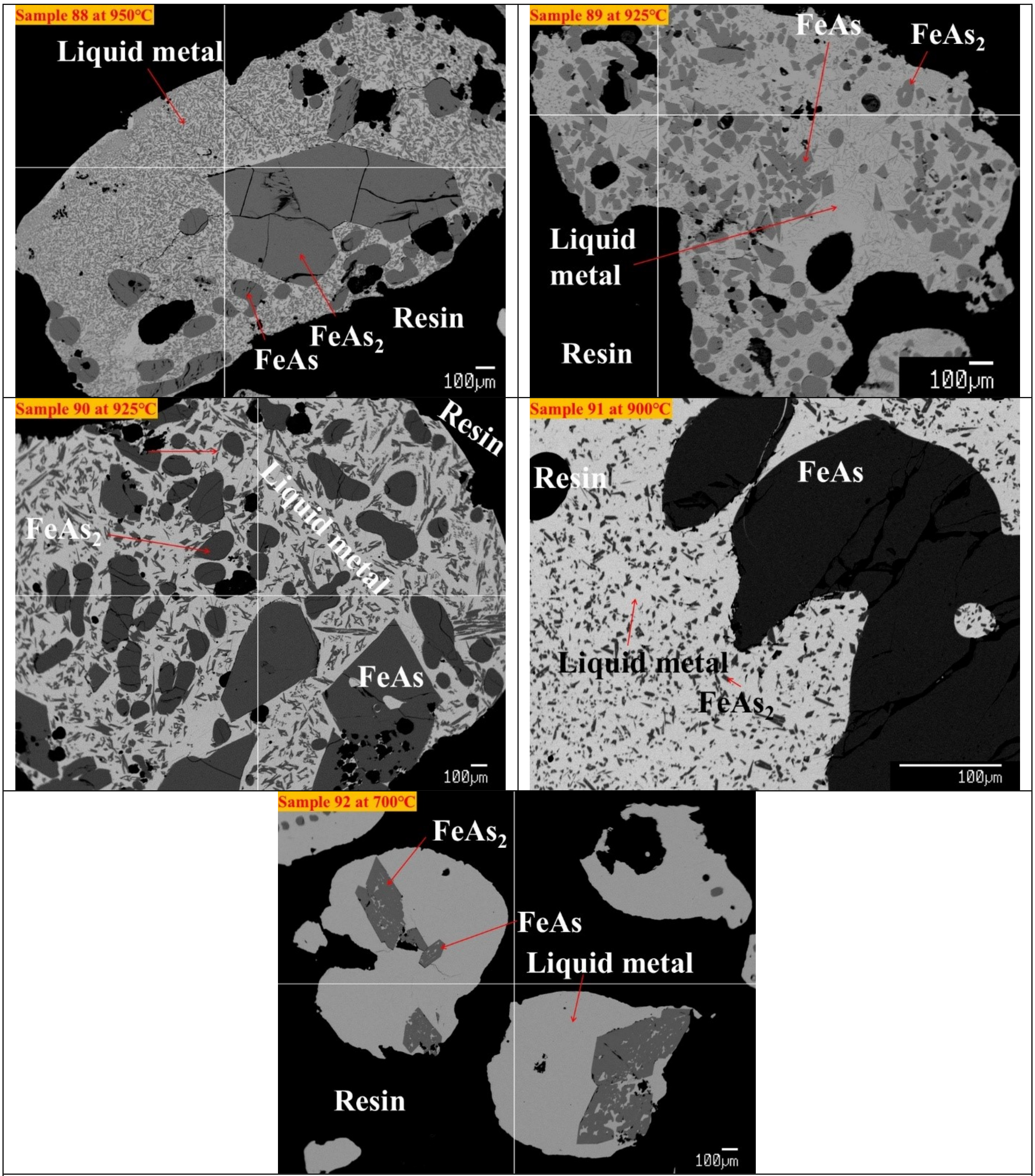
(g) Boundary between MeX-Fe_{1+x}(Sb, As) and Fe(As, Sb) primary phase fields (Sample 86)



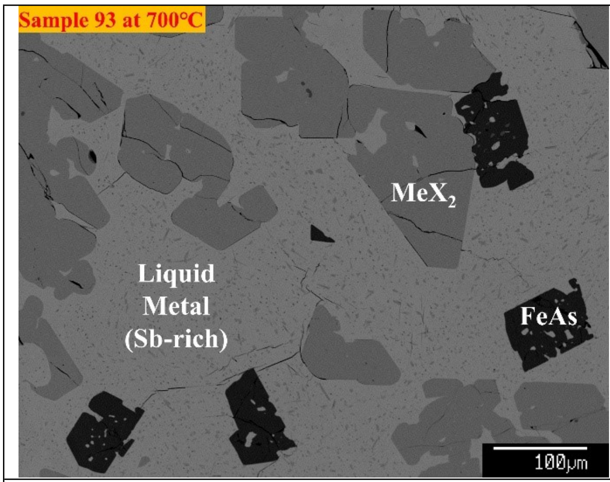
(h) Boundary between MeX-Fe_{1+x}(Sb, As) and Fe_2(As, Sb) primary phase fields (Sample 87)

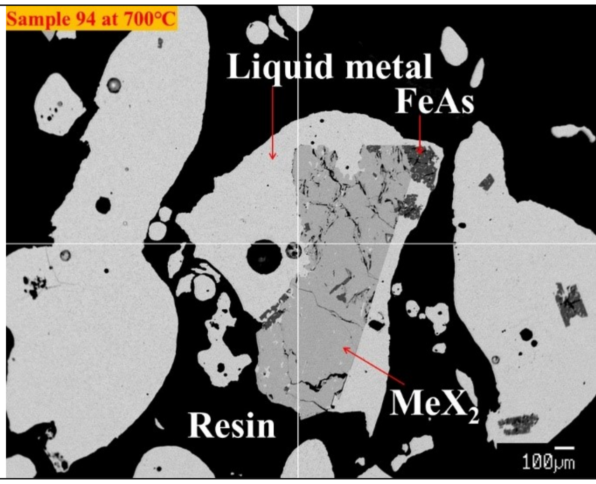


(i) Boundary between Fe(As, Sb) and Fe(As, Sb)$_2$ primary phase fields (Sample 88-92)

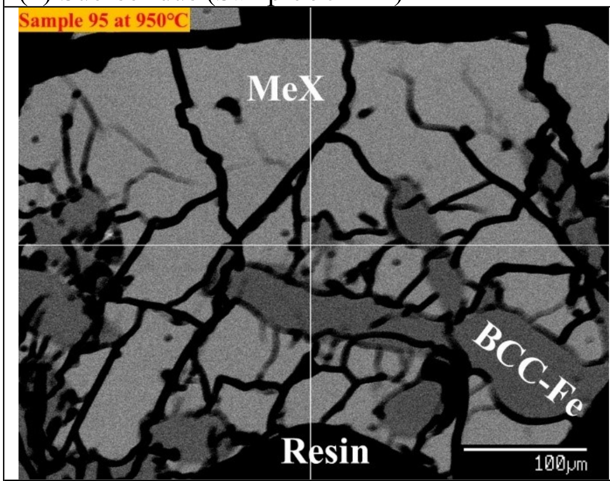


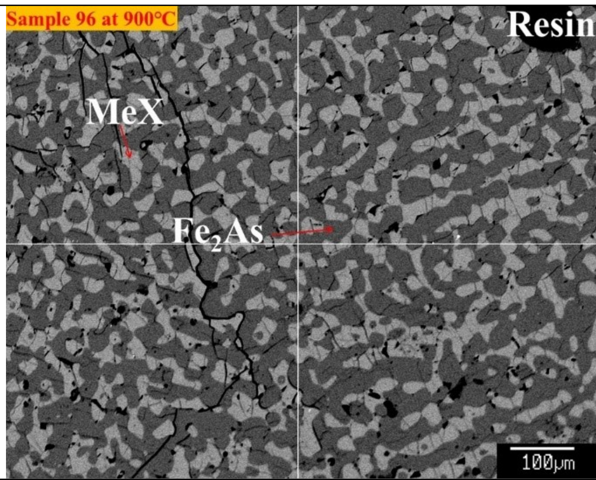
(j) Boundary between Fe(As, Sb) and MeX_2 (Me = Fe and X = Sb and As) primary phase fields (Sample 93-94)

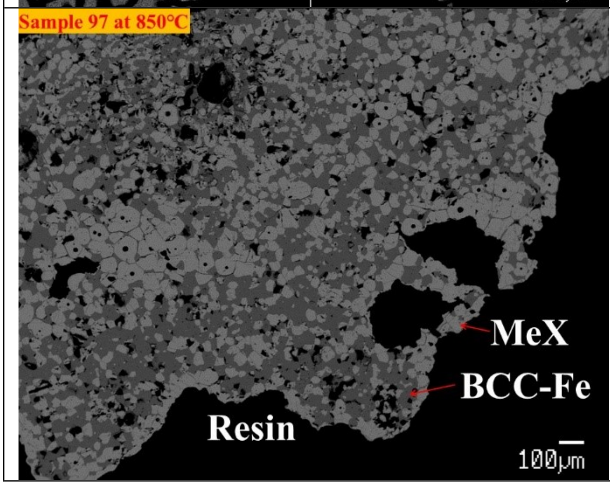


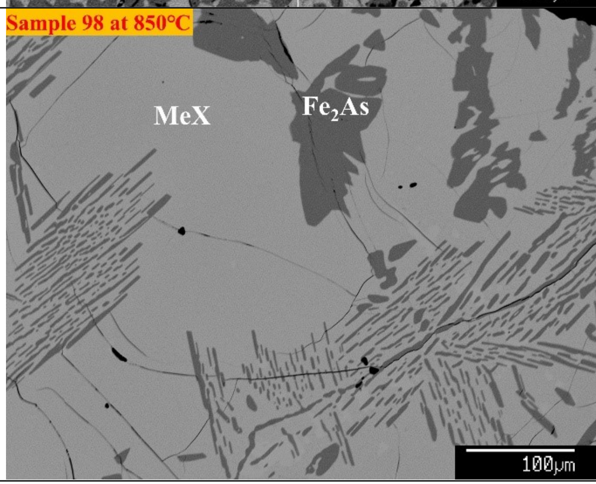


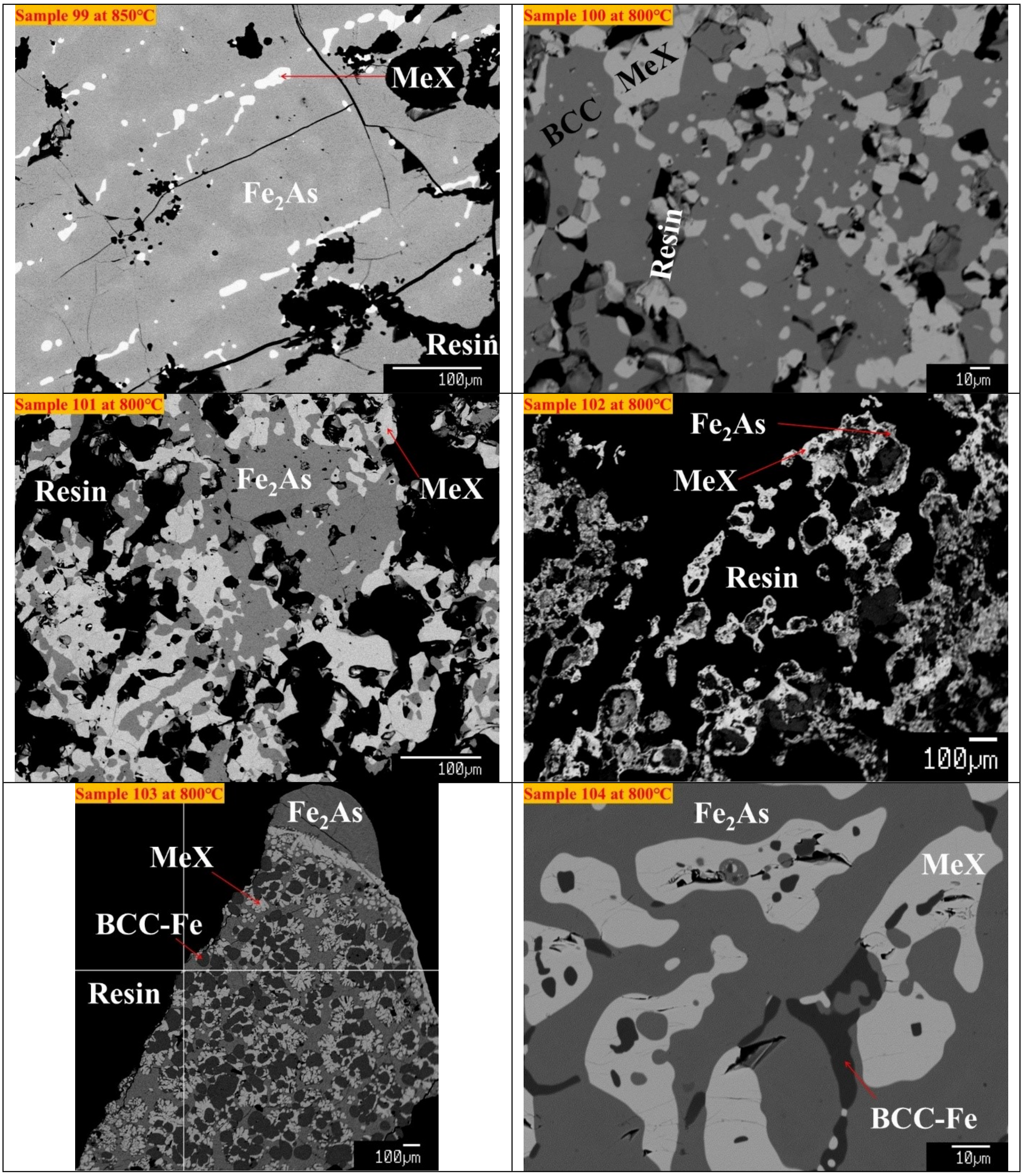
(k) Sub-solidus (Sample 95-112)

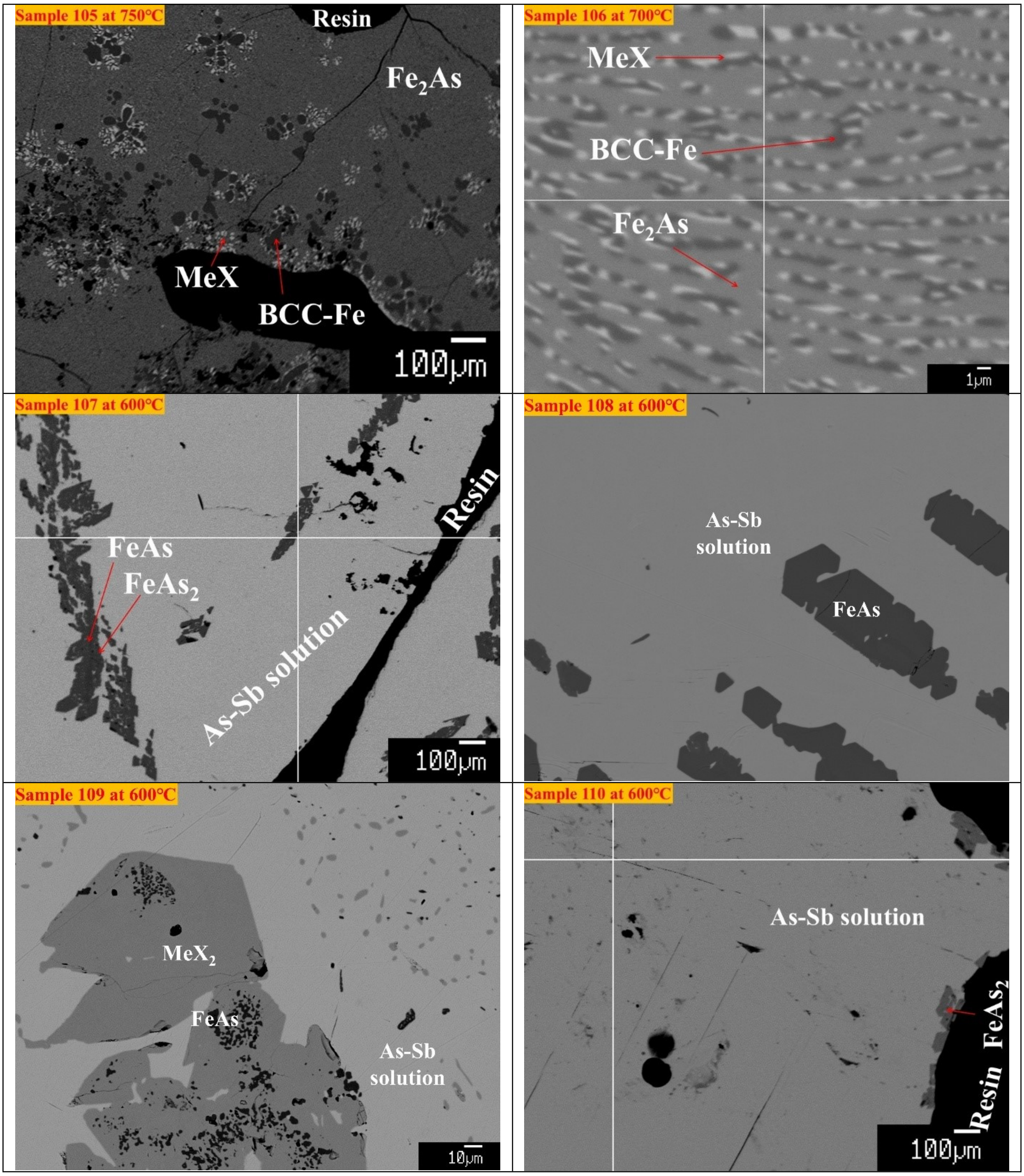









Sample 99 at 850°C
MeX
Fe2As
Resin
100μm
Sample 100 at 800°C
MeX
BCC
Resin
10μm
Sample 101 at 800°C
Resin
Fe2As
MeX
100μm
Sample 102 at 800°C
Fe2As
MeX
Resin
100μm
Sample 103 at 800°C
Fe2As
MeX
BCC-Fe
Resin
100μm
Sample 104 at 800°C
Fe2As
MeX
BCC-Fe
10μm



Sample 105 at 750°C
Resin
Fe2As
MeX
BCC-Fe
100μm
Sample 106 at 700°C
MeX
BCC-Fe
Fe2As
1μm
Sample 107 at 600°C
Resin
FeAs
FeAs2
As-Sb solution
100μm
Sample 108 at 600°C
As-Sb solution
FeAs
Sample 109 at 600°C
MeX2
FeAs
As-Sb solution
10μm
Sample 110 at 600°C
As-Sb solution
FeAs2
Resin
100μm

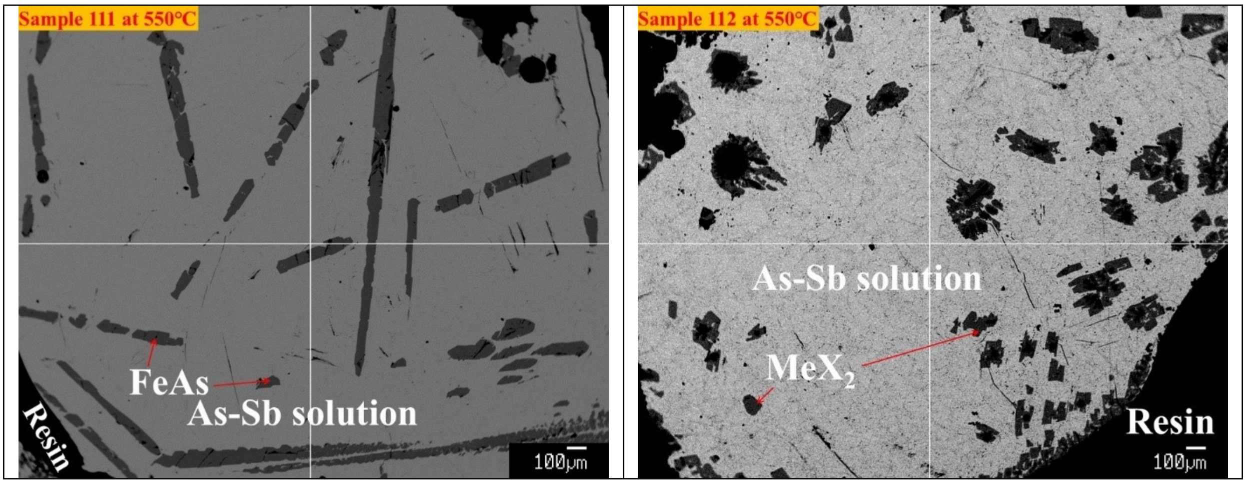
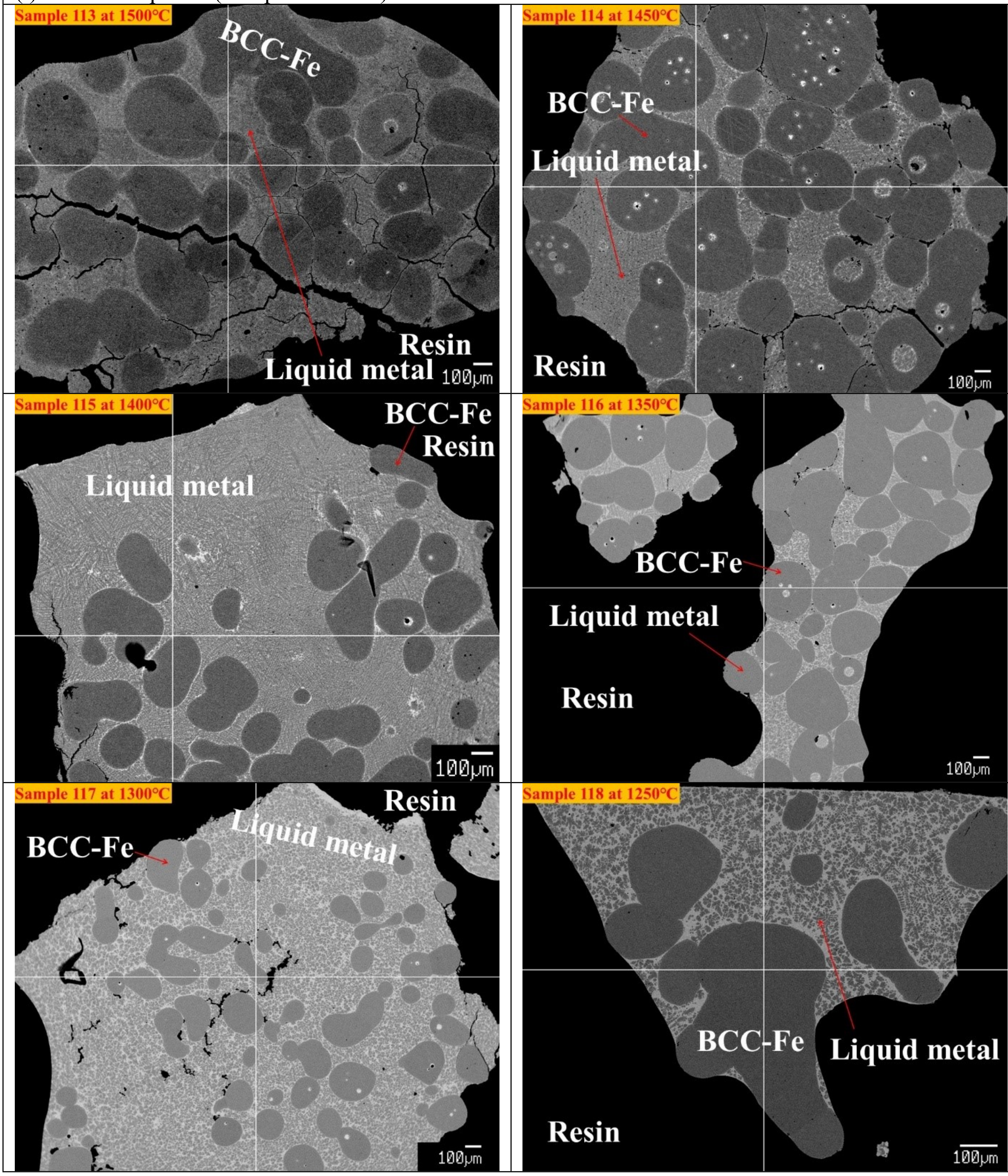
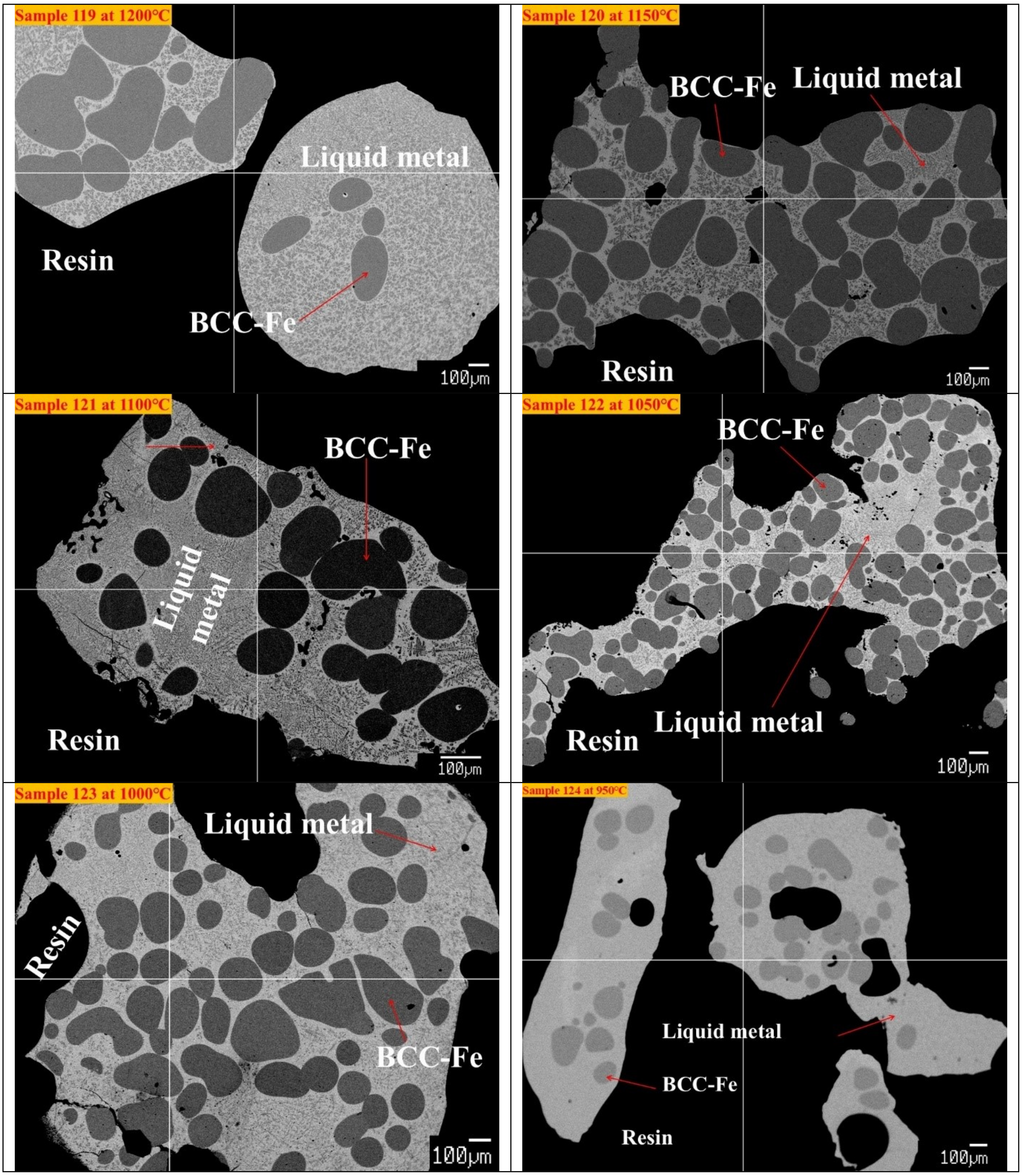


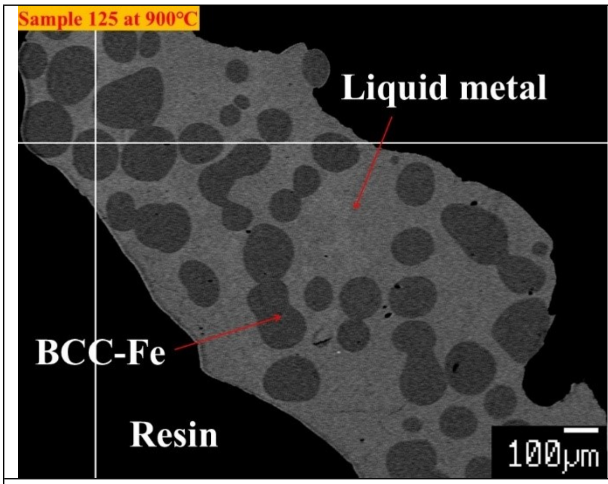
Figure S1 Microstructures for the Fe-Sb-As systems in the same chronological order with phases given in Table S1.

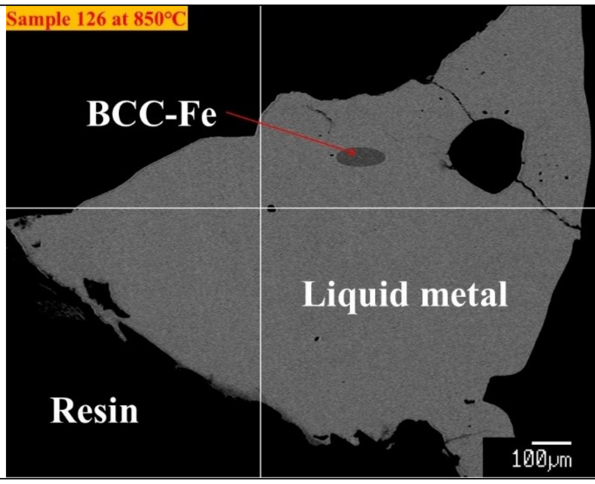
(l) BCC-Fe liquidus (Sample 113-126)



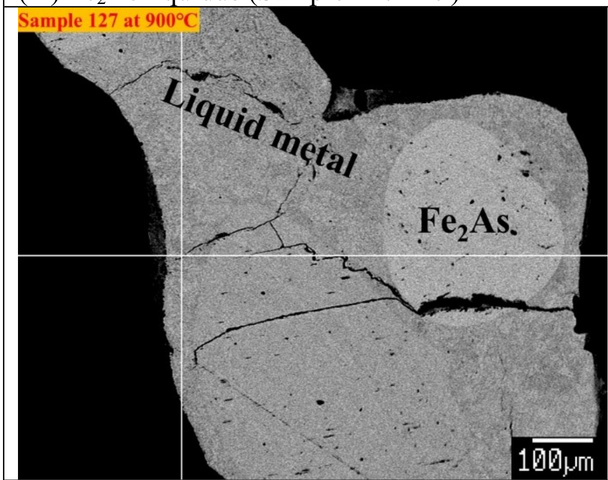


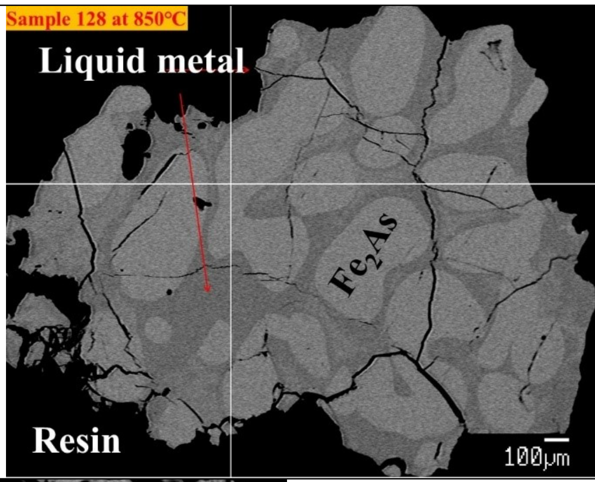
Sample 119 at 1200°C
Liquid metal
Resin
BCC-Fe
100μm
Sample 120 at 1150°C
BCC-Fe
Liquid metal
Resin
100μm
Sample 121 at 1100°C
BCC-Fe
Liquid metal
Resin
100μm
Sample 122 at 1050°C
BCC-Fe
Liquid metal
Resin
100μm
Sample 123 at 1000°C
Liquid metal
Resin
BCC-Fe
100μm
Sample 124 at 950°C
Liquid metal
BCC-Fe
Resin
100μm

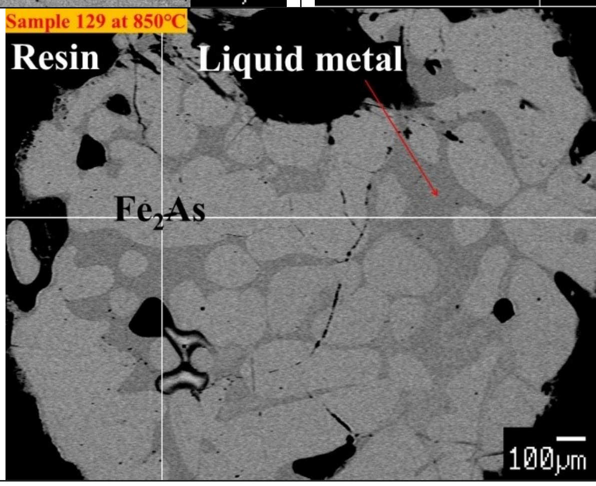




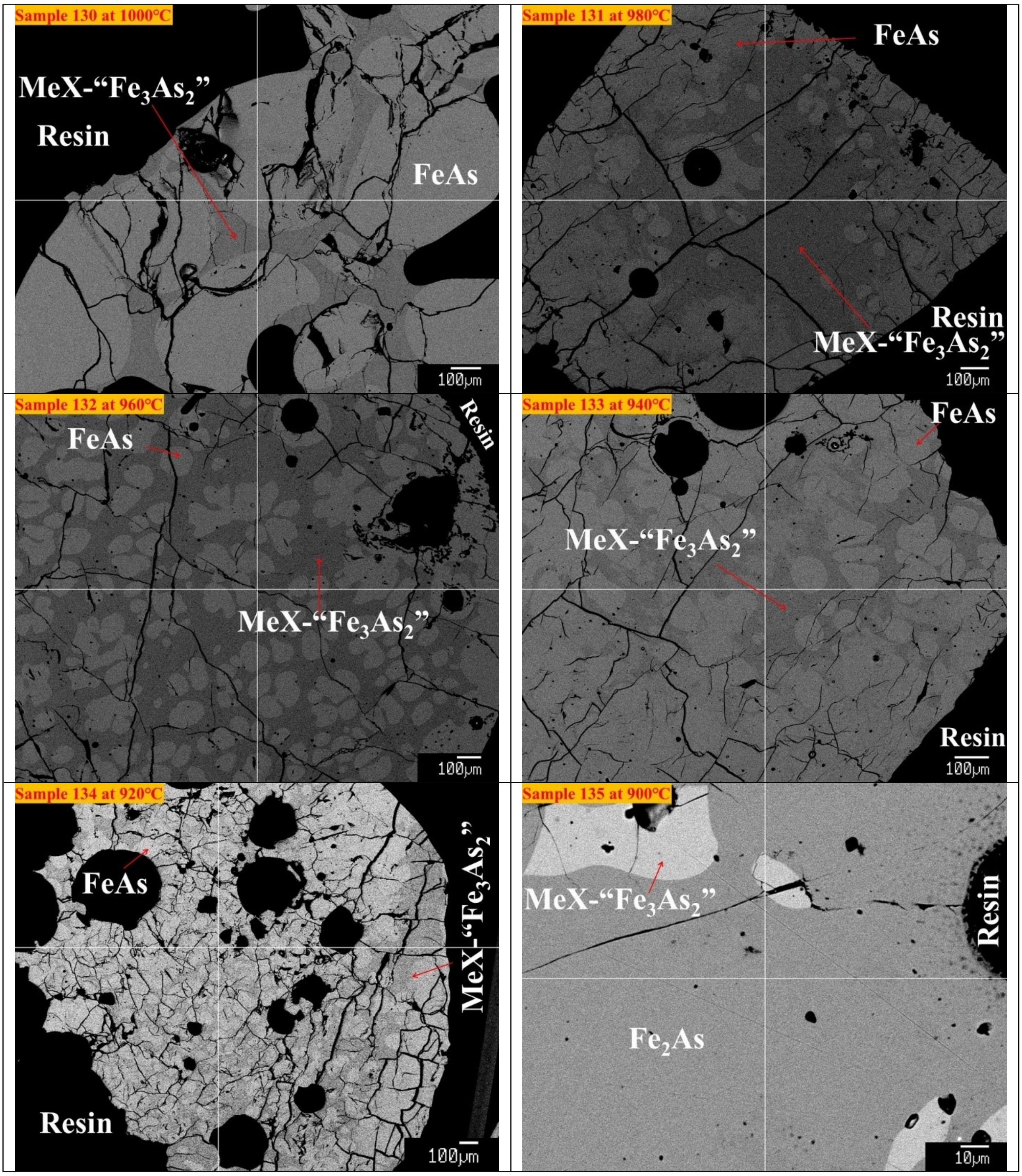
(m) Fe_2As liquidus (Sample 127-129)



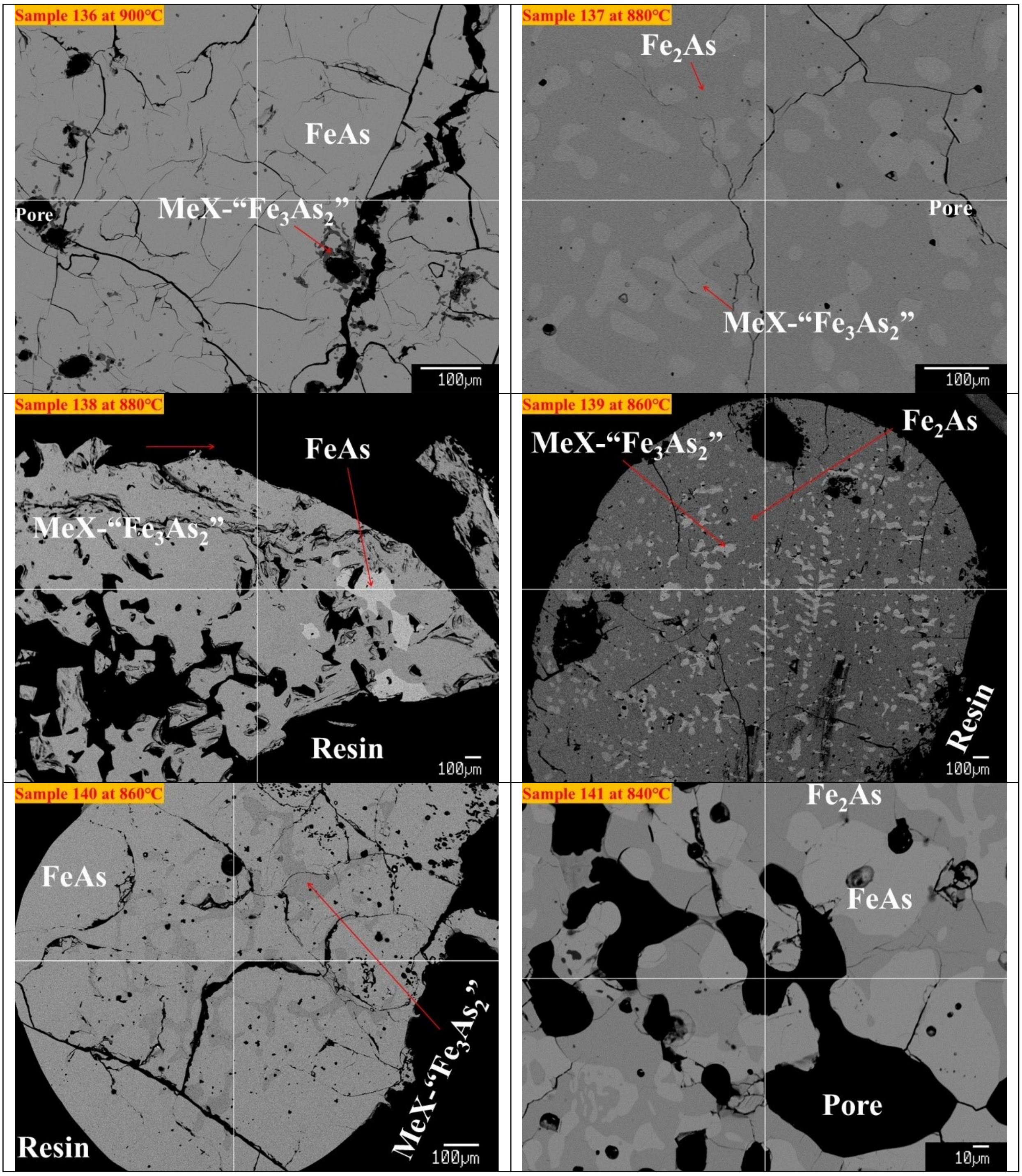




(n) Sub-solidus (Sample 130-146)



Sample 130 at 1000°C
MeX-"Fe_3As_2"
Resin
FeAs
100μm
Sample 131 at 980°C
FeAs
Resin
MeX-"Fe_3As_2"
100μm
Sample 132 at 960°C
Resin
FeAs
MeX-"Fe_3As_2"
100μm
Sample 133 at 940°C
FeAs
MeX-"Fe_3As_2"
Resin
100μm
Sample 134 at 920°C
FeAs
MeX-"Fe_3As_2"
Resin
100μm
Sample 135 at 900°C
MeX-"Fe_3As_2"
Resin
Fe_2As
10μm



Sample 136 at 900°C
FeAs
Pore
MeX-"Fe_3As_2"
100μm
Sample 137 at 880°C
Fe_2As
Pore
MeX-"Fe_3As_2"
100μm
Sample 138 at 880°C
FeAs
MeX-"Fe_3As_2"
Resin
100μm
Sample 139 at 860°C
Fe_2As
MeX-"Fe_3As_2"
Resin
100μm
Sample 140 at 860°C
FeAs
MeX-"Fe_3As_2"
Resin
100μm
Sample 141 at 840°C
Fe_2As
FeAs
Pore
10μm

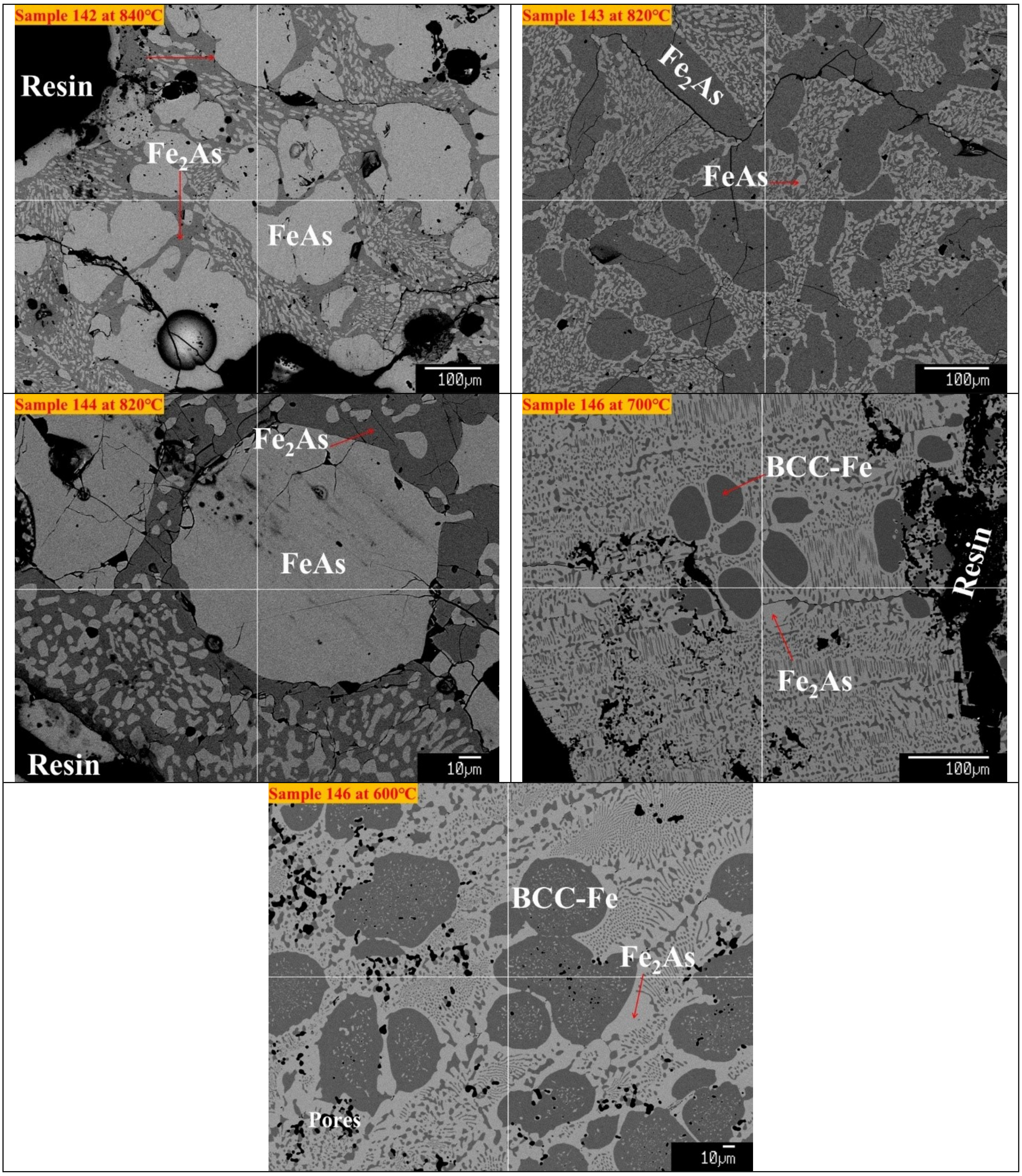
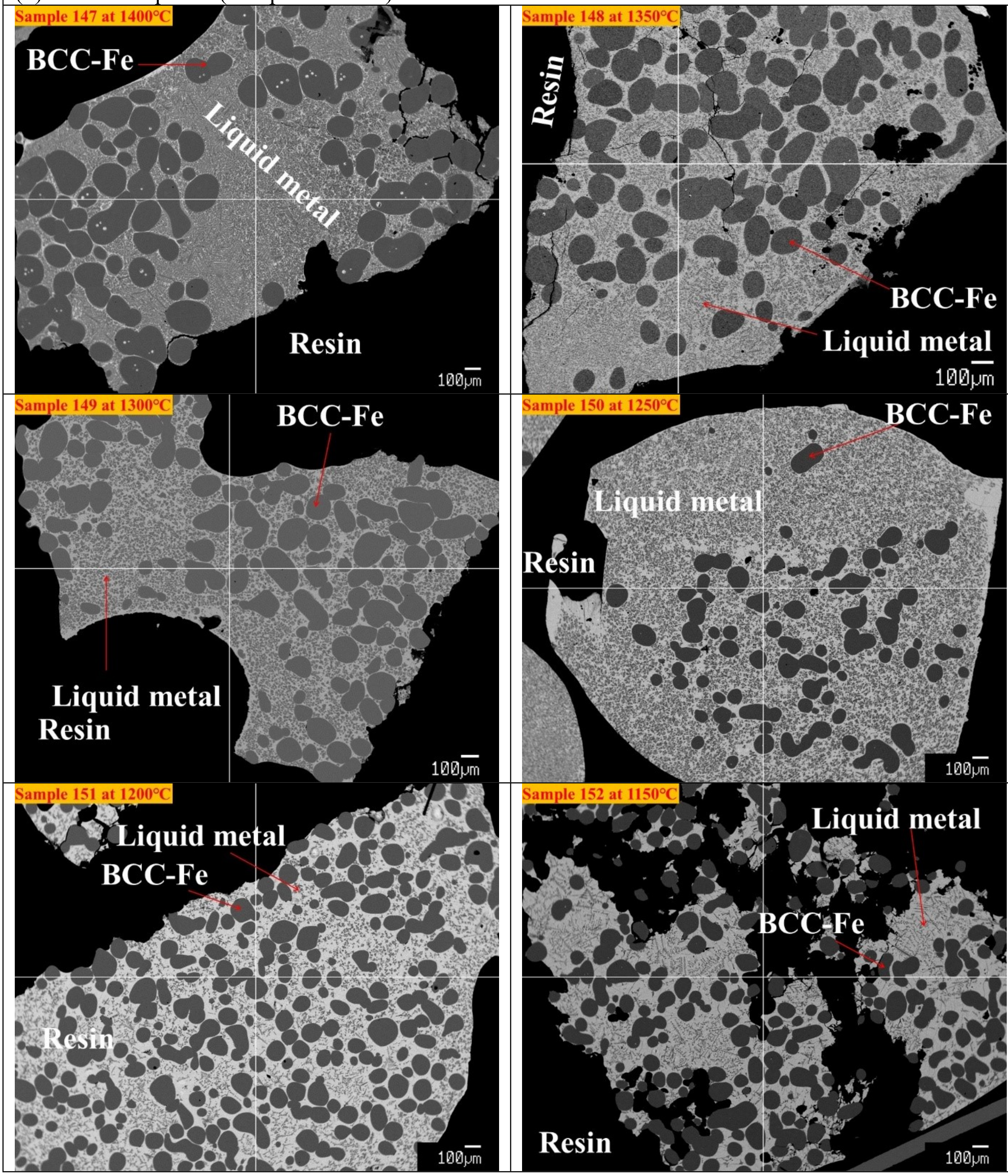
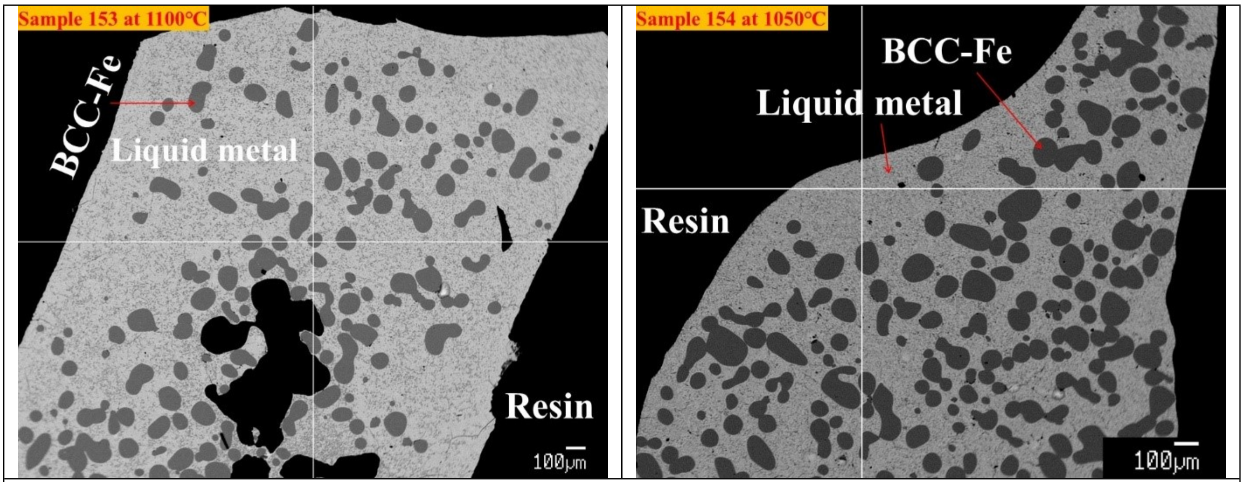


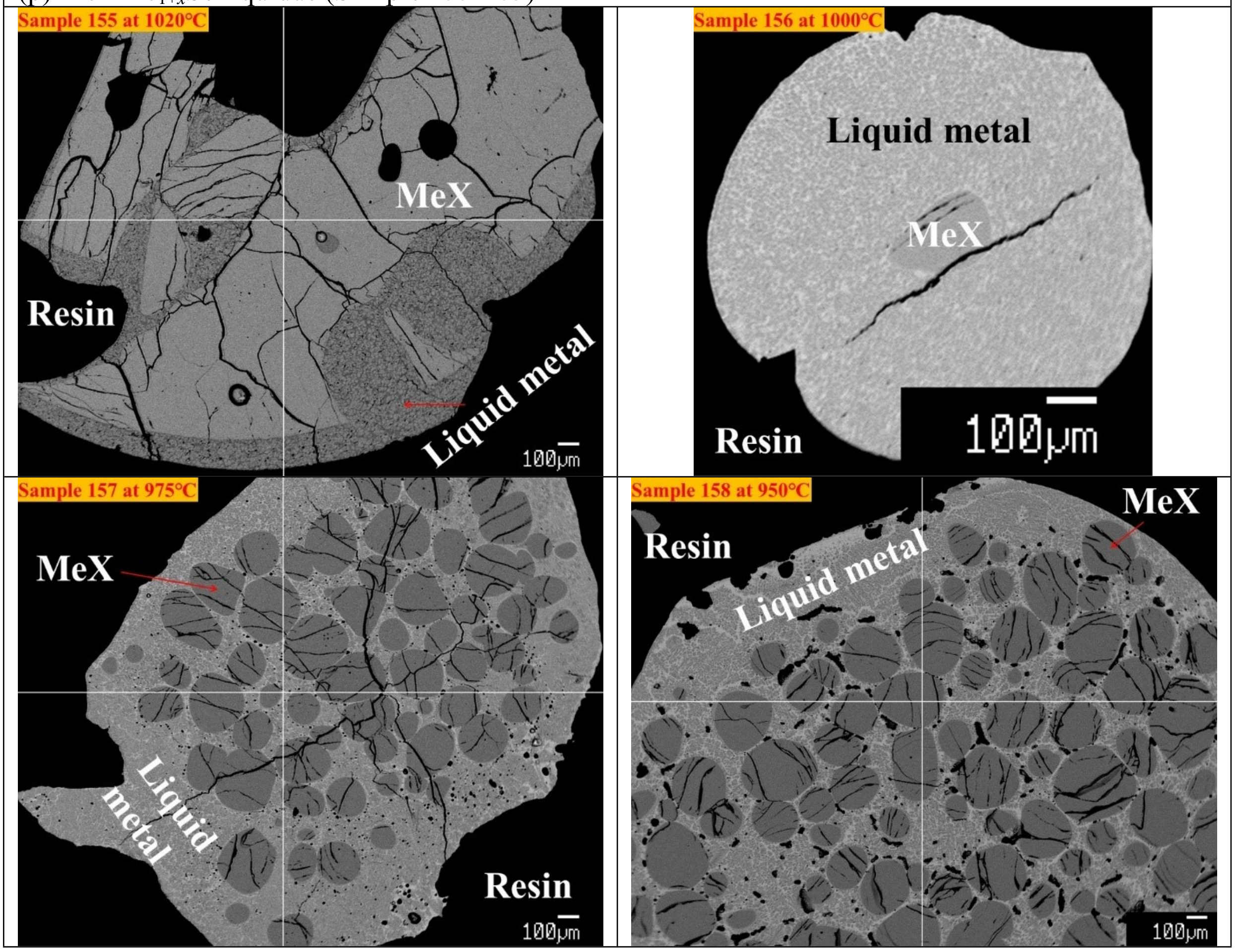
Figure S2 Microstructures for the Fe-As systems in the same chronological order given in Table S2.

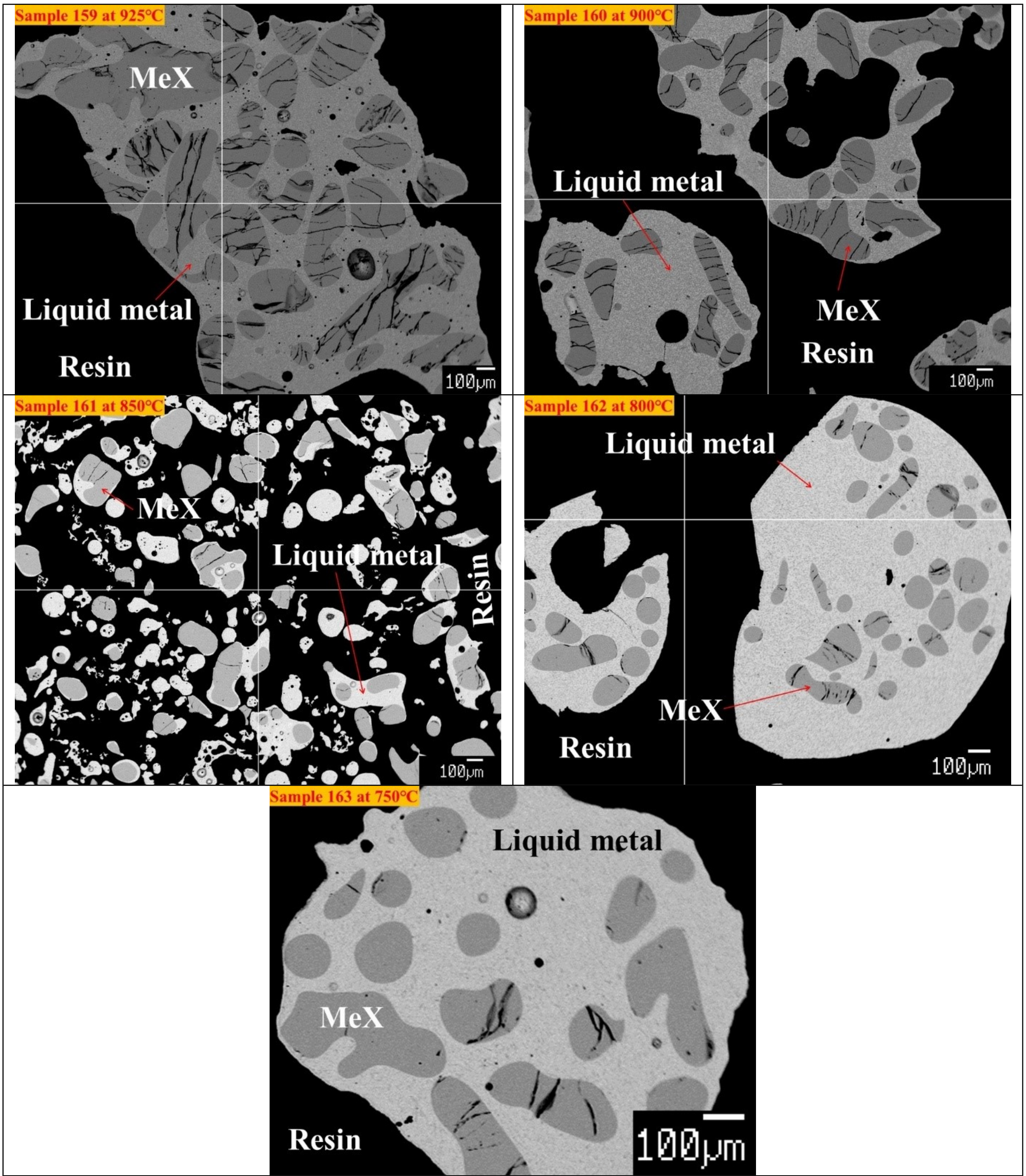
(o) BCC-Fe liquidus (Sample 147-154)



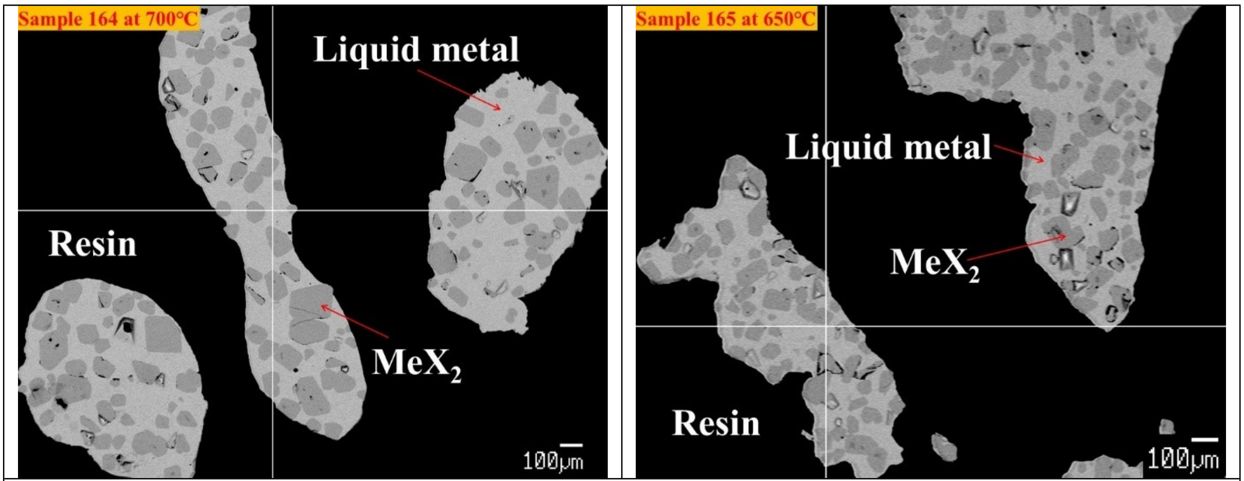


(p) MeX-$Fe_{1+x}Sb$ liquidus (Sample 155-163)





(q) MeX_2 (Me = Fe and X = Sb) liquidus (Sample 164-165)



(r) Sub-solidus (Sample 166-167)

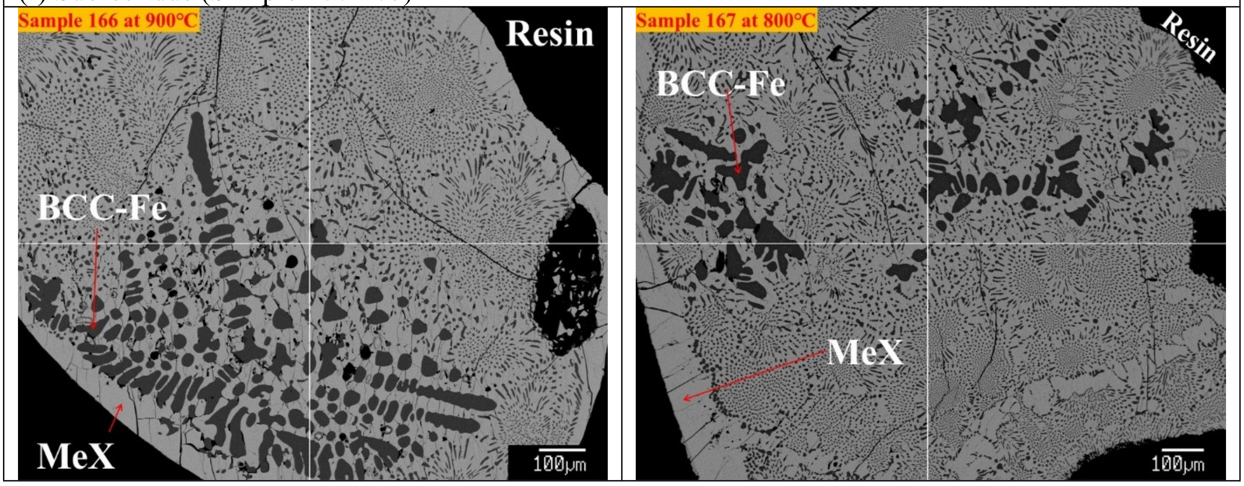


Figure S3 Microstructures for the Fe-Sb systems in the same chronological order given in Table S3.

Table S1 Measured composition of the phases (average values and standard deviation) in the Fe-Sb-As system, expressed in mol.% with SiO_2 substrate of each phase equilibrated at fixed temperature and fixed first preheating at 600 °C for 1 h to all arsenic containing samples with or without second preheating.

S. no.	Preheat 2 (°C/h)	Equilibration		Phase	Normalized mol. %			Unnormalized (wt.%)
		T (°C)	t (h)		Fe	Sb	As	
(a) BCC-Fe liquidus								
1	-	1000	7	Liquid metal	68.4 ± 0.2	28.3 ± 0.2	3.4 ± 0.0	100.33
				BCC-Fe	94.1 ± 0.1	4.0 ± 0.0	1.9 ± 0.1	100.20
2	-	1000	4.75	Liquid metal	69.7 ± 0.1	24.4 ± 0.1	5.9 ± 0.1	100.33
				BCC-Fe	93.6 ± 0.0	3.1 ± 0.0	3.3 ± 0.0	100.32
3	-	950	4	Liquid metal	71.0 ± 0.2	16.5 ± 0.2	12.5 ± 0.2	100.33
				BCC-Fe	92.5 ± 0.0	1.9 ± 0.0	5.6 ± 0.0	100.36
(b) MeX = Fe_{1+x}(Sb, As) liquidus								
4	-	1000	6	Liquid metal	65.2 ± 0.7	30.9 ± 0.9	4.0 ± 0.2	100.38
				MeX	59.1 ± 0.2	39.3 ± 0.2	1.6 ± 0.1	99.72
5	-	950	5.5	Liquid metal	39.7 ± 2.3	55.6 ± 2.5	4.7 ± 0.3	100.12
				MeX	54.4 ± 0.2	41.2 ± 0.2	4.4 ± 0.1	99.92
6	-	950	5.5	Liquid metal	43.0 ± 0.9	26.4 ± 1.5	30.6 ± 0.7	100.06
				MeX	53.8 ± 0.1	6.2 ± 0.1	40.0 ± 0.2	100.21
7	-	950	6	Liquid metal	68.5 ± 0.5	18.2 ± 0.7	13.3 ± 0.7	100.26
				MeX	57.9 ± 0.1	35.4 ± 0.1	6.7 ± 0.0	100.07
8	-	950	4.25	Liquid metal	48.7 ± 1.2	38.1 ± 1.4	13.1 ± 0.3	100.09
				MeX	55.4 ± 0.2	31.0 ± 0.2	13.6 ± 0.1	100.29
9	-	950	4.25	Liquid metal	43.9 ± 0.9	47.1 ± 1.1	9.0 ± 0.2	100.17
				MeX	55.0 ± 0.2	34.7 ± 0.1	10.3 ± 0.1	99.65
10	-	950	12.25	Liquid metal	48.8 ± 0.7	20.8 ± 1.0	30.4 ± 0.4	100.31
				MeX	55.0 ± 0.1	10.2 ± 0.1	34.8 ± 0.1	100.18
11	1000/0.5	925	19.75	Liquid metal	38.7 ± 0.4	48.4 ± 0.6	12.9 ± 0.3	100.29
				MeX	55.1 ± 0.2	24.1 ± 0.1	20.8 ± 0.1	100.17
12	1000/0.5	925	20	Liquid metal	39.1 ± 0.6	37.6 ± 1.0	23.4 ± 0.4	100.16
				MeX	54.8 ± 0.1	11.9 ± 0.1	33.3 ± 0.1	100.26
13	1000/0.5	925	20.75	Liquid metal	28.1 ± 1.0	47.5 ± 1.5	24.4 ± 0.6	100.28
				MeX	52.9 ± 0.1	7.3 ± 0.0	39.8 ± 0.1	100.32
14	-	925	25.5	Liquid metal	42.1 ± 0.4	40.0 ± 0.5	18.0 ± 0.4	100.13
				MeX	55.3 ± 0.1	20.7 ± 0.1	24.0 ± 0.1	100.30
15	1000/0.5	900	4	Liquid metal	27.0 ± 0.8	64.5 ± 1.4	8.5 ± 0.8	100.16
				MeX	55.0 ± 0.5	24.0 ± 0.3	21.0 ± 0.2	100.11
16	1000/0.5	900	15	Liquid metal	20.1 ± 0.9	65.8 ± 1.4	14.2 ± 0.6	100.13
				MeX	53.8 ± 0.1	10.7 ± 0.1	35.5 ± 0.1	100.22
17	1000/0.5	900	6	Liquid metal	29.5 ± 1.0	67.6 ± 1.0	2.9 ± 0.1	100.23
				MeX	53.6 ± 0.2	41.9 ± 0.2	4.5 ± 0.1	100.38
18	1000/0.5	900	20	Liquid metal	66.0 ± 0.2	8.8 ± 0.2	25.2 ± 0.1	100.35
				MeX	59.0 ± 0.1	19.0 ± 0.1	22.1 ± 0.1	100.20
19	1000/0.5	850	12	Liquid metal	21.6 ± 2.3	71.9 ± 3.3	6.5 ± 1.0	100.21
				MeX	53.8 ± 0.1	25.7 ± 0.3	20.5 ± 0.3	100.09
20	950/0.5	850	15	Liquid metal	14.5 ± 0.7	76.6 ± 1.2	8.9 ± 0.6	100.29
				MeX	53.0 ± 0.1	14.8 ± 0.2	32.2 ± 0.1	100.19
21	1000/0.5	850	8	Liquid metal	12.8 ± 0.7	77.4 ± 1.0	9.7 ± 0.9	100.39
				MeX	52.5 ± 0.1	9.8 ± 1.2	37.7 ± 1.2	100.12
22	1000/0.5	850	6.5	Liquid metal	13.1 ± 0.7	77.3 ± 1.1	9.6 ± 0.5	100.29
				MeX	53.0 ± 0.1	11.7 ± 0.1	35.3 ± 0.0	100.34

23	1000/0.5	850	13.5	Liquid metal	22.6 ± 0.7	74.9 ± 0.7	2.5 ± 0.1	99.84
				MeX	53.7 ± 0.1	39.4 ± 0.1	6.9 ± 0.1	100.09
24	1000/0.5	850	21	Liquid metal	22.2 ± 0.8	74.6 ± 0.8	3.2 ± 0.1	99.77
				MeX	53.7 ± 0.1	39.7 ± 0.1	6.6 ± 0.0	100.26
25	900/0.5	800	13	Liquid metal	13.8 ± 0.7	82.7 ± 1.0	3.5 ± 0.3	100.26
				MeX	53.1 ± 0.1	26.6 ± 0.6	20.2 ± 0.5	100.24
26	-	800	11	Liquid metal	9.3 ± 2.1	84.9 ± 2.5	5.8 ± 1.7	100.15
				MeX	52.2 ± 0.4	21.1 ± 0.7	26.7 ± 1.1	100.34
27	1000/0.5	800	6	Liquid metal	16.9 ± 1.2	81.2 ± 1.3	1.9 ± 0.1	100.20
				MeX	53.2 ± 0.2	42.4 ± 0.1	4.5 ± 0.1	100.24
28	1000/0.5	750	43	Liquid metal	9.7 ± 0.2	88.2 ± 0.2	2.1 ± 0.1	100.22
				MeX	52.4 ± 0.1	31.3 ± 0.2	16.3 ± 0.3	100.26
29	1000/0	750	6	Liquid metal	8.0 ± 0.6	89.2 ± 0.8	2.8 ± 0.3	100.43
				MeX	52.4 ± 0.1	22.2 ± 0.5	25.4 ± 0.5	100.33
(c) Fe(As, Sb) liquidus								
30	-	1000	5	Liquid metal	39.4 ± 0.7	13.3 ± 1.2	47.3 ± 1.2	100.42
				FeAs	49.4 ± 0.1	0.43 ± 0.01	50.2 ± 0.1	100.98
31	-	975	7	Liquid metal	27.5 ± 1.0	28.3 ± 1.4	44.2 ± 0.6	100.17
				FeAs	50.2 ± 0.1	0.06 ± 0.01	49.7 ± 0.1	100.72
32	-	975	4.5	Liquid metal	42.5 ± 0.7	20.3 ± 1.0	37.2 ± 0.5	100.30
				FeAs	50.5 ± 0.1	0.94 ± 0.11	48.6 ± 0.1	100.84
33	-	975	6.5	Liquid metal	27.5 ± 0.8	31.9 ± 1.2	40.6 ± 0.9	100.09
				FeAs	50.1 ± 0.2	0.15 ± 0.01	49.8 ± 0.2	100.04
34	-	975	5	Liquid metal	30.5 ± 0.6	32.8 ± 0.9	36.7 ± 0.5	100.31
				FeAs	49.6 ± 0.1	0.90 ± 0.02	49.6 ± 0.1	100.86
35	-	975	5	Liquid metal	28.7 ± 2.8	22.9 ± 3.7	48.3 ± 1.4	100.32
				FeAs	49.5 ± 0.1	0.39 ± 0.02	50.1 ± 0.1	100.79
36	1000/0.5	950	20.5	Liquid metal	34.1 ± 0.7	35.7 ± 1.1	30.3 ± 0.6	100.18
				FeAs	49.0 ± 0.2	1.5 ± 0.0	49.5 ± 0.2	100.09
37	1000/0.5	950	21.5	Liquid metal	19.0 ± 1.3	42.6 ± 2.2	38.4 ± 1.0	100.31
				FeAs	49.5 ± 0.2	0.55 ± 0.01	50.0 ± 0.2	100.68
38	1000/0.5	950	21	Liquid metal	20.3 ± 1.4	45.7 ± 2.2	34.1 ± 0.8	100.34
				FeAs	49.5 ± 0.1	0.73 ± 0.01	49.8 ± 0.1	100.38
39	-	950	5	Liquid metal	21.4 ± 0.7	46.4 ± 1.1	32.2 ± 0.4	100.42
				FeAs	49.7 ± 0.1	0.85 ± 0.02	49.5 ± 0.1	100.84
40	1000/0.5	950	22	Liquid metal	21.8 ± 2.1	46.4 ± 3.8	31.8 ± 1.8	100.22
				FeAs	49.8 ± 0.2	0.87 ± 0.02	49.3 ± 0.2	100.50
41	-	950	5.75	Liquid metal	28.3 ± 1.8	42.4 ± 3.4	29.3 ± 1.8	100.13
				FeAs	50.1 ± 0.1	0.80 ± 0.05	49.1 ± 0.1	100.20
42	-	950	5.75	Liquid metal	18.8 ± 1.7	37.7 ± 1.3	43.5 ± 3.0	100.37
				FeAs	49.7 ± 0.1	0.33 ± 0.02	50.0 ± 0.1	100.93
43	-	950	5.25	Liquid metal	19.8 ± 1.1	32.1 ± 2.6	48.1 ± 2.1	100.44
				FeAS	49.3 ± 0.1	0.38 ± 0.03	50.3 ± 0.1	100.83
44	-	925	5.5	Liquid metal	26.6 ± 0.8	49.8 ± 1.3	23.6 ± 0.6	100.32
				FeAs	49.8 ± 0.4	1.3 ± 0.0	49.0 ± 0.4	100.47
45	-	925	6	Liquid metal	10.8 ± 0.9	53.7 ± 0.8	35.5 ± 0.7	100.31
				FeAs	50.0 ± 0.1	0.00 ± 0.00	50.0 ± 0.1	100.89
46	-	925	5	Liquid metal	13.6 ± 0.5	64.3 ± 0.9	22.1 ± 0.5	100.22
				FeAs	50.2 ± 0.2	0.56 ± 0.03	49.2 ± 0.2	100.25
47	1000/0.5	925	20.75	Liquid metal	18.3 ± 0.9	62.5 ± 1.7	19.2 ± 0.9	100.43
				FeAs	50.0 ± 0.1	1.7 ± 0.3	48.3 ± 0.3	100.22
48	1000/0.5	925	20	Liquid metal	12.3 ± 0.8	62.5 ± 1.1	25.3 ± 0.6	100.40
				FeAs	49.6 ± 0.1	0.79 ± 0.02	49.6 ± 0.1	100.82

49	1000/0.5	925	19.75	Liquid metal	10.8 ± 0.6	50.7 ± 1.1	38.5 ± 0.8	100.30
				FeAs	49.8 ± 0.1	0.37 ± 0.01	49.9 ± 0.1	100.21
50	1000/0.5	900	14	Liquid metal	17.2 ± 0.5	67.3 ± 0.9	15.5 ± 0.5	100.10
				FeAs	49.7 ± 0.1	1.9 ± 0.1	48.4 ± 0.1	100.33
51	950/0.5	900	58	Liquid metal	7.7 ± 0.6	72.0 ± 1.2	20.3 ± 0.7	100.05
				FeAs	49.8 ± 0.1	0.80 ± 0.04	49.4 ± 0.1	99.97
52	1000/0.5	900	21	Liquid metal	9.0 ± 0.7	73.0 ± 1.4	18.0 ± 0.7	100.09
				FeAs	49.7 ± 0.2	0.89 ± 0.02	49.5 ± 0.2	100.76
53	-	850	36	Liquid metal	5.3 ± 0.3	79.8 ± 0.7	14.9 ± 0.4	100.18
				FeAs	49.8 ± 0.1	0.61 ± 0.03	49.6 ± 0.1	100.34
54	1000/0.5	850	8	Liquid metal	6.5 ± 0.9	80.6 ± 1.8	12.9 ± 0.9	100.23
				FeAs	49.8 ± 0.1	1.1 ± 0.1	49.1 ± 0.1	100.67
55	-	800	10	Liquid metal	2.8 ± 0.4	82.8 ± 0.9	14.5 ± 0.6	100.26
				FeAs	49.4 ± 0.2	0.36 ± 0.04	50.3 ± 0.2	100.74
56	1000/0.5	800	4.5	Liquid metal	2.4 ± 0.3	82.1 ± 0.5	15.5 ± 0.3	100.32
				FeAs	49.0 ± 0.1	0.61 ± 0.06	50.4 ± 0.2	100.30
57	1000/0.5	800	11.5	Liquid metal	5.5 ± 0.6	86.3 ± 1.4	8.2 ± 0.8	100.32
				FeAs	49.9 ± 0.1	1.4 ± 0.3	48.7 ± 0.2	100.62
58	850/0.5	750	56	Liquid metal	1.2 ± 0.2	86.4 ± 0.7	12.4 ± 0.7	99.66
				FeAs	49.7 ± 0.1	0.35 ± 0.08	49.9 ± 0.1	100.48
59	1000/0.5	750	12.5	Liquid metal	3.8 ± 0.2	91.6 ± 0.3	4.6 ± 0.2	100.43
				FeAs	49.8 ± 0.1	1.1 ± 0.1	49.1 ± 0.2	101.00
60	1000/0.5	700	13.5	Liquid metal	1.4 ± 0.1	92.4 ± 0.2	6.2 ± 0.1	100.28
				FeAs	49.5 ± 0.2	0.60 ± 0.30	49.9 ± 0.3	100.65
61	1000/0.5	650	10.25	Liquid metal	1.3 ± 0.1	95.2 ± 0.1	3.5 ± 0.1	100.15
				FeAs	50.1 ± 0.2	0.66 ± 0.23	49.3 ± 0.2	100.36
(d) $Fe(As, Sb)_2$ liquidus								
62	-	900	5.5	Liquid metal	6.7 ± 0.5	58.8 ± 0.9	34.4 ± 0.9	100.29
				$FeAs_2$	33.3 ± 0.1	1.2 ± 0.1	65.5 ± 0.2	101.00
63	1000/0.5	850	19	Liquid metal	3.9 ± 0.6	72.0 ± 1.3	24.1 ± 0.9	100.36
				$FeAs_2$	32.9 ± 0.1	1.3 ± 0.2	65.8 ± 0.2	100.13
64	1000/0.5	850	36.5	Liquid metal	2.7 ± 0.3	65.3 ± 0.8	32.1 ± 0.5	100.29
				$FeAs_2$	33.2 ± 0.2	0.92 ± 0.22	65.9 ± 0.2	100.91
65	1000/0.5	850	18.5	Liquid metal	3.4 ± 0.3	70.8 ± 0.7	25.8 ± 0.4	100.12
				$FeAs_2$	33.2 ± 0.1	0.85 ± 0.13	65.9 ± 0.2	100.91
66	-	850	42	Liquid metal	2.8 ± 0.1	66.5 ± 0.4	30.7 ± 0.3	100.42
				$FeAs_2$	33.6 ± 0.1	0.77 ± 0.05	65.7 ± 0.2	100.05
67	1000/0.5	800	14	Liquid metal	2.0 ± 0.2	79.7 ± 0.5	18.2 ± 0.4	100.17
				$FeAs_2$	32.8 ± 0.1	1.3 ± 0.2	65.9 ± 0.1	100.25
68	1000/0.5	800	36.5	Liquid metal	1.1 ± 0.1	68.9 ± 0.4	30.1 ± 0.4	99.83
				$FeAs_2$	33.5 ± 0.1	0.80 ± 0.23	65.7 ± 0.3	100.53
69	1000/0.5	800	13.5	Liquid metal	1.8 ± 0.5	76.5 ± 0.6	21.7 ± 0.3	100.42
				$FeAs_2$	32.8 ± 0.2	1.0 ± 0.2	66.1 ± 0.3	101.02
70	-	800	16	Liquid metal	1.0 ± 0.8	66.6 ± 0.8	32.5 ± 0.6	99.87
				$FeAs_2$	33.1 ± 0.1	0.44 ± 0.02	66.4 ± 0.1	100.99
71	1000/0.5	800	6.5	Liquid metal	1.1 ± 0.1	70.5 ± 0.3	28.3 ± 0.2	100.25
				$FeAs_2$	33.4 ± 0.4	0.99 ± 0.82	65.6 ± 0.4	100.38
72	1000/0.5	750	39	Liquid metal	1.1 ± 0.2	85.3 ± 0.6	13.6 ± 0.4	100.16
				$FeAs_2$	33.3 ± 0.1	1.4 ± 0.1	65.3 ± 0.1	100.51
73	850/0.5	750	13	Liquid metal	0.60 ± 0.11	78.0 ± 0.3	21.4 ± 0.2	99.62
				$FeAs_2$	33.6 ± 0.2	0.26 ± 0.19	66.1 ± 0.2	100.67
74	1000/5mi	750	42	Liquid metal	0.46 ±	74.1 ± 0.2	25.4 ± 0.2	100.22

	n.				0.07			
				$FeAs_2$	33.4 ± 0.1	0.62 ± 0.39	66.0 ± 0.4	100.86
75	1000/5min.	700	14.5	Liquid metal	0.94 ± 0.11	90.7 ± 0.1	8.3 ± 0.1	100.33
				$FeAs_2$	33.5 ± 0.1	1.8 ± 0.3	64.7 ± 0.3	99.99
76	1000/0.5	700	11.5	Liquid metal	0.36 ± 0.08	78.9 ± 0.3	20.7 ± 0.2	100.14
				$FeAs_2$	33.2 ± 0.0	1.1 ± 0.5	65.7 ± 0.5	100.41
77	800/0.5	700	14.25	Liquid metal	0.50 ± 0.11	80.0 ± 0.5	19.5 ± 0.4	99.71
				$FeAs_2$	33.2 ± 0.5	1.04 ± 0.37	65.7 ± 0.4	100.61
78	950/0.5	650	12	Liquid metal	0.52 ± 0.07	89.9 ± 0.3	9.6 ± 0.3	99.67
				$FeAs_2$	33.6 ± 0.0	0.36 ± 0.35	66.1 ± 0.4	100.59
79	850/0.5	650	15	Liquid metal	0.27 ± 0.14	79.2 ± 0.5	20.5 ± 0.3	99.71
				$FeAs_2$	33.5 ± 0.1	0.49 ± 0.55	66.0 ± 0.6	100.50
80	800/0.5	650	10.5	Liquid metal	0.25 ± 0.06	79.3 ± 0.1	20.4 ± 0.1	99.79
				$FeAs_2$	33.3 ± 0.1	0.34 ± 0.42	66.4 ± 0.4	100.39
(e) MeX_2 (Me = Fe and X = Sb and As) liquidus								
81	1000/0.5	650	36.5	Liquid metal	2.2 ± 0.2	96.1 ± 0.3	1.7 ± 0.1	100.00
				MeX_2	33.6 ± 0.1	60.5 ± 0.1	5.9 ± 0.1	100.36
(f) Boundary between BCC-Fe and MeX = Fe_{1+x}(Sb, As) primary phase fields								
82	-	975	6.5	Liquid metal	68.9 ± 0.4	24.2 ± 0.6	7.0 ± 0.4	100.34
				BCC-Fe	93.6 ± 0.1	3.0 ± 0.0	3.4 ± 0.0	100.40
				MeX	59.7 ± 0.1	37.8 ± 0.1	2.4 ± 0.0	100.31
83	1000/0.5	900	4	Liquid metal	71.7 ± 0.2	11.4 ± 0.1	16.9 ± 0.2	100.08
				BCC-Fe	91.5 ± 0.0	1.3 ± 0.0	7.1 ± 0.0	99.96
				MeX	59.0 ± 0.0	32.8 ± 0.1	8.1 ± 0.1	99.69
84	950/0.5	900	10.75	Liquid metal	72.3 ± 0.5	10.2 ± 0.3	17.5 ± 0.6	100.33
				BCC-Fe	91.4 ± 0.2	1.3 ± 0.1	7.3 ± 0.1	100.26
				MeX	59.8 ± 0.2	31.6 ± 0.1	8.6 ± 0.1	100.19
85	1000/0.5	850	10.25	Liquid metal	72.0 ± 0.1	7.8 ± 0.1	20.3 ± 0.1	100.18
				BCC-Fe	91.0 ± 0.1	0.86 ± 0.02	8.1 ± 0.1	100.28
				MeX	60.0 ± 0.1	27.5 ± 0.1	12.5 ± 0.0	100.40
(g) Boundary between MeX = Fe_{1+x}(Sb, As) and Fe(As, Sb) primary phase fields								
86	1000/0.5	750	36	Liquid metal	6.2 ± 0.6	90.6 ± 0.9	3.2 ± 0.3	100.32
				MeX	51.9 ± 0.1	18.8 ± 0.4	29.3 ± 0.4	100.29
				FeAs	49.5 ± 0.3	2.6 ± 0.1	47.9 ± 0.3	101.01
(h) Boundary between MeX = Fe_{1+x}(Sb, As) and Fe_2(As, Sb)								
87	950/0.5	850	13.5	Liquid metal	69.3 ± 0.5	6.0 ± 0.1	24.7 ± 0.5	100.16
				MeX	59.8 ± 0.2	19.5 ± 0.1	20.7 ± 0.1	99.76
				Fe_2As	65.8 ± 0.1	2.6 ± 0.1	31.6 ± 0.1	100.12
(i) Boundary between Fe(As, Sb) and $Fe(As, Sb)_2$ primary phase fields								
88	-	950	6	Liquid metal	20.3 ± 0.9	30.7 ± 1.4	49.0 ± 0.8	100.44
				FeAs	49.7 ± 0.1	0	50.3 ± 0.1	100.20
				$FeAs_2$	33.6 ± 0.1	0.15 ± 0.06	66.3 ± 0.2	100.91
89	-	925	5.5	Liquid metal	10.6 ± 0.4	50.2 ± 1.0	39.2 ± 1.0	100.43
				FeAs	50.1 ± 0.0	0	49.9 ± 0.0	100.30
				$FeAs_2$	34.0 ± 0.1	0.33 ± 0.07	65.6 ± 0.1	100.90
90	1000/0.5	925	14.25	Liquid metal	11.0 ± 0.5	48.5 ± 1.2	40.5 ± 0.9	100.45
				FeAs	49.8 ± 0.2	0.36 ± 0.02	49.8 ± 0.2	100.13

				$FeAs_2$	33.4 ± 0.2	1.0 ± 0.2	65.5 ± 0.1	100.67
91	1000/0.5	900	14	Liquid metal	6.8 ± 0.3	60.8 ± 0.9	32.4 ± 0.9	100.35
				FeAs	49.6 ± 0.2	0.48 ± 0.09	50.0 ± 0.2	99.85
				$FeAs_2$	32.3 ± 0.7	2.1 ± 0.8	65.6 ± 0.2	100.51
92	1000/0.5	700	12	Liquid metal	1.0 ± 0.2	90.8 ± 0.2	8.1 ± 0.1	100.23
				FeAs	49.3 ± 0.1	0.44 ± 0.17	50.3 ± 0.2	100.74
				$FeAs_2$	32.8 ± 0.1	1.7 ± 0.2	65.6 ± 0.1	100.87
(j) Boundary between Fe(As, Sb) and MeX_2 (Me = Fe and X = Sb and As) primary phase fields								
93	1000/0.5	700	20	Liquid metal	4.8 ± 0.5	93.3 ± 0.5	1.9 ± 0.1	100.28
				FeAs	50.4 ± 0.1	2.9 ± 0.2	46.8 ± 0.3	100.71
				MeX_2	33.7 ± 0.1	61.6 ± 0.1	4.7 ± 0.1	99.78
94	1000/0.5	700	6	Liquid metal	4.7 ± 0.5	93.4 ± 0.5	1.9 ± 0.1	100.15
				FeAs	49.2 ± 1.2	2.5 ± 0.2	48.3 ± 1.3	100.30
				MeX_2	33.7 ± 0.2	59.5 ± 0.7	6.7 ± 0.6	100.35
(k) Sub-solidus								
95	1000/0.5	950	21	MeX	53.5 ± 0.1	5.1 ± 0.1	41.4 ± 0.1	100.32
				FeAs	49.8 ± 0.2	0.84 ± 0.07	49.3 ± 0.2	100.78
96	1000/0.5	900	24	Fe_2As	65.5 ± 0.2	0.88 ± 0.02	33.6 ± 0.2	100.14
				MeX	59.4 ± 0.8	4.6 ± 0.5	36.0 ± 0.3	100.43
97	900/0.5	850	12	BCC-Fe	91.0 ± 0.0	0.76 ± 0.01	8.3 ± 0.0	99.80
				MeX	59.6 ± 0.1	28.0 ± 0.0	12.4 ± 0.1	100.26
98	1000/0.5	850	12	MeX	60.9 ± 0.8	6.1 ± 0.9	33.0 ± 0.0	100.22
				Fe_2As	65.1 ± 0.1	1.4 ± 0.0	33.5 ± 0.1	100.17
99	1000/0.5	850	15	MeX	60.2 ± 0.3	19.2 ± 0.2	20.5 ± 0.2	100.31
				Fe_2As	65.9 ± 0.1	1.4 ± 0.5	32.7 ± 0.4	100.06
100	900/0.5	800	5	BCC-Fe	91.3 ± 0.1	0.58 ± 0.02	8.1 ± 0.1	100.06
				MeX	59.3 ± 0.1	28.3 ± 0.1	12.4 ± 0.0	100.32
101	900/0.5	800	14	MeX	57.4 ± 0.3	10.2 ± 0.1	32.4 ± 0.3	100.33
				Fe_2As	65.7 ± 0.1	1.3 ± 0.1	32.9 ± 0.2	100.20
102	900/0.5	800	17	MeX	54.9 ± 0.4	11.2 ± 0.1	33.8 ± 0.4	99.95
				FeAs	49.9 ± 0.2	1.8 ± 0.2	48.3 ± 0.4	100.82
103	1000/0.5	800	5	BCC-Fe	90.5 ± 0.5	0.93 ± 0.39	8.6 ± 0.1	100.42
				MeX	60.1 ± 0.2	25.1 ± 0.6	14.8 ± 0.4	100.23
				Fe_2As	68.7 ± 0.5	3.0 ± 0.1	28.3 ± 0.4	100.32
104	950/0.5	800	15	BCC-Fe	90.6 ± 0.3	0.70 ± 0.12	8.6 ± 0.2	99.66
				MeX	59.5 ± 0.1	26.2 ± 0.0	14.3 ± 0.1	99.67
				Fe_2As	65.8 ± 0.1	2.8 ± 0.1	31.5 ± 0.1	100.08
105	950/0.5	750	15	BCC-Fe	91.5 ± 0.1	0.49 ± 0.02	8.0 ± 0.1	99.78
				MeX	58.7 ± 0.2	29.5 ± 0.2	11.9 ± 0.1	100.12
				Fe_2As	65.9 ± 0.1	3.2 ± 0.1	30.9 ± 0.1	100.09
106	950/0.5	700	12	BCC-Fe	92.0 ± 0.1	0.45 ± 0.04	7.5 ± 0.0	100.13
				MeX	58.0 ± 0.2	31.9 ± 0.5	10.1 ± 0.5	100.28
				Fe_2As	66.5 ± 0.8	2.8 ± 0.2	30.7 ± 0.7	100.27
107	950/0.5	600	11.5	FeAs	50.4 ± 0.2	0.06 ± 0.01	49.6 ± 0.2	100.33
				$FeAs_2$	33.6 ± 0.2	0.88 ± 0.24	65.5 ± 0.3	100.19
				As-Sb solution	0.0 ± 0.1	90.2 ± 1.1	9.8 ± 1.1	99.67
108	1000/0.5	600	10.5	FeAs	50.1 ± 0.1	0.60 ± 0.52	49.3 ± 0.6	100.48
				As-Sb solution	0.3 ± 0.2	95.9 ± 0.8	3.8 ± 0.7	99.83
109	900/0.5	600	38	FeAs	49.2 ± 0.4	1.7 ± 0.7	49.1 ± 0.4	100.70
				MeX_2	33.6 ± 0.2	60.2 ± 0.7	6.3 ± 0.7	100.39
				As-Sb	1.1 ± 0.6	97.8 ± 0.9	1.1 ± 0.3	99.86

				solution				
110	800/0.5	600	12	$FeAs_2$	33.5 ± 0.3	0.21 ± 0.26	66.3 ± 0.5	100.52
				As-Sb solution	0.0 ± 0.1	78.1 ± 0.3	21.9 ± 0.3	99.77
111	1000/0.5	550	37	FeAs	50.6 ± 0.2	1.1 ± 0.2	48.3 ± 0.3	100.46
				As-Sb solution	0.4 ± 0.2	97.4 ± 0.5	2.2 ± 0.3	99.90
112	900/0.5	550	37	MeX_2	33.8 ± 0.2	60.0 ± 0.7	6.2 ± 0.6	100.33
				As-Sb solution	0.9 ± 0.4	98.0 ± 0.7	1.1 ± 0.3	99.71

Table S2 Measured composition of the phases (average values and standard deviation) in the Fe-As system, expressed in mol.% with SiO_2 substrate of each phase equilibrated at fixed temperature and fixed first preheating at 600 °C for 1 h to all arsenic containing samples with or without second preheating.

S. no.	Preheat 2 (°C/h)	Equilibration		Phase	Normalized mol. %		Unnormalized (wt.%)
		T (°C)	t (h)		Fe	As	
(l) BCC-Fe liquidus							
113	-	1500	3	Liquid metal	97.2 ± 0.2	2.8 ± 0.2	100.02
				BCC-Fe	99.19 ± 0.02	0.81 ± 0.02	99.75
114	-	1450	5.25	Liquid metal	93.9 ± 0.1	6.1 ± 0.1	100.48
				BCC-Fe	98.1 ± 0.0	1.9 ± 0.0	99.71
115	-	1400	4.75	Liquid metal	91.1 ± 0.1	8.9 ± 0.1	100.24
				BCC-Fe	97.2 ± 0.1	2.8 ± 0.1	99.76
116	-	1350	13.5	Liquid metal	88.8 ± 0.2	11.2 ± 0.2	100.33
				BCC-Fe	96.4 ± 0.0	3.6 ± 0.0	99.87
117	-	1300	11.5	Liquid metal	86.5 ± 0.4	13.5 ± 0.4	100.34
				BCC-Fe	95.5 ± 0.0	4.5 ± 0.0	99.93
118	-	1250	25.5	Liquid metal	84.1 ± 0.6	15.9 ± 0.6	100.50
				BCC-Fe	94.8 ± 0.2	5.2 ± 0.2	99.79
119	-	1200	26.5	Liquid metal	81.7 ± 0.4	18.3 ± 0.4	100.31
				BCC-Fe	93.9 ± 0.2	6.1 ± 0.2	99.92
120	-	1150	18.75	Liquid metal	80.8 ± 0.6	19.2 ± 0.6	100.13
				BCC-Fe	93.3 ± 0.1	6.7 ± 0.1	99.84
121	-	1100	5.75	Liquid metal	79.1 ± 0.3	20.9 ± 0.3	100.01
				BCC-Fe	92.8 ± 0.1	7.2 ± 0.1	100.05
122	-	1050	5.75	Liquid metal	77.7 ± 0.4	22.3 ± 0.4	100.32
				BCC-Fe	92.3 ± 0.1	7.7 ± 0.1	100.12
123	-	1000	25.5	Liquid metal	76.7 ± 0.5	23.3 ± 0.5	100.11
				BCC-Fe	91.6 ± 0.1	8.4 ± 0.1	100.03
124	1000/0.5	950	17	Liquid metal	75.8 ± 0.3	24.2 ± 0.3	100.26
				BCC-Fe	91.1 ± 0.1	8.9 ± 0.1	99.90
125	1000/0.5	900	15.75	Liquid metal	75.1 ± 0.2	24.9 ± 0.2	100.24
				BCC-Fe	90.7 ± 0.1	9.3 ± 0.1	100.07
126	1000/0.5	850	47.25	Liquid metal	74.3 ± 0.2	25.7 ± 0.2	100.34
				BCC-Fe	90.3 ± 0.1	9.7 ± 0.1	100.13
(m) Fe_2As liquidus							
127	1000/0.5	900	24.5	Liquid metal	69.5 ± 0.3	30.5 ± 0.2	100.20
				Fe_2As	66.2 ± 0.2	33.8 ± 0.2	100.41
128	1000/0.5	850	40	Liquid metal	74.0 ± 0.2	26.0 ± 0.0	99.90
				Fe_2As	66.4 ± 0.0	33.6 ± 0.0	100.13
129	1000/0.5	850	7.25	Liquid metal	74.0 ± 0.2	26.0 ± 0.0	99.90
				Fe_2As	66.3 ± 0.2	33.7 ± 0.0	99.98
(n) Sub-solidus							
130	-	1000	72.75	FeAs	49.8 ± 0.1	50.2 ± 0.1	100.19
				MeX "Fe_3As_2"	55.3 ± 0.1	44.7 ± 0.1	100.45
131	1050/0.25	980	71.75	FeAs	49.9 ± 0.1	50.1 ± 0.0	100.66
				MeX "Fe_3As_2"	55.8 ± 0.2	44.2 ± 0.1	100.49
132	1050/0.25	960	84.75	FeAs	50.0 ± 0.1	50.0 ± 0.1	100.48
				MeX "Fe_3As_2"	56.7 ± 0.1	43.3 ± 0.1	100.12
133	1050/0.2	940	70.7	FeAs	50.1 ± 0.0	49.9 ± 0.2	100.66

	5		5	MeX “Fe_3As_2”	57.1 ± 0.1	42.9 ± 0.1	100.07
134	1050/0.25	920	72	FeAs	49.8 ± 0.1	50.2 ± 0.2	100.84
				MeX “Fe_3As_2”	57.1 ± 0.1	42.9 ± 0.1	100.10
135	1000/0.5	900	75	Fe_2As	66.4 ± 0.2	33.6 ± 0.2	100.26
				MeX “Fe_3As_2”	59.7 ± 0.1	40.3 ± 0.1	100.54
136	1050/0.25	900	71.5	FeAs	49.8 ± 0.2	50.2 ± 0.1	100.86
				MeX “Fe_3As_2”	57.5 ± 0.1	42.5 ± 0.1	100.19
137	1000/0.5	880	71.5	Fe_2As	66.6 ± 0.2	33.4 ± 0.1	100.14
				MeX “Fe_3As_2”	59.3 ± 0.1	40.7 ± 0.1	100.12
138	1050/0.25	880	71	FeAs	50.3 ± 0.1	49.7 ± 0.1	100.07
				MeX “Fe_3As_2”	58.1 ± 0.1	41.9 ± 0.1	100.04
139	1000/0.5	860	85.5	Fe_2As	66.4 ± 0.1	33.6 ± 0.1	100.28
				MeX “Fe_3As_2”	59.2 ± 0.1	40.8 ± 0.1	100.37
140	1050/0.25	860	84	FeAs	49.9 ± 0.1	50.1 ± 0.1	100.20
				MeX “Fe_3As_2”	58.4 ± 0.1	41.6 ± 0.1	100.50
141	1000/0.5	840	94.5	Fe_2As	66.3 ± 0.1	33.7 ± 0.1	100.38
				FeAs	49.9 ± 0.1	50.1 ± 0.0	100.75
142	1050/0.25	840	70.5	Fe_2As	66.4 ± 0.1	33.6 ± 0.1	100.03
				FeAs	49.9 ± 0.1	50.1 ± 0.0	101.00
143	1000/0.5	820	72.75	Fe_2As	66.3 ± 0.1	33.7 ± 0.0	100.12
				FeAs	50.2 ± 0.0	49.8 ± 0.0	100.12
144	1050/0.25	820	74.5	Fe_2As	66.6 ± 0.1	33.4 ± 0.0	100.16
				FeAs	50.0 ± 0.0	50.0 ± 0.0	100.15
145	1000/0.5	700	86	BCC-Fe	91.8 ± 0.1	8.2 ± 0.0	100.19
				Fe_2As	66.2 ± 0.1	33.8 ± 0.0	100.30
146	1000/0.5	600	85	BCC-Fe	92.3 ± 0.4	7.7 ± 0.0	99.62
				Fe_2As	66.1 ± 0.2	33.9 ± 0.0	100.27

Table S3 Measured composition of the phases (average values and standard deviation) in the Fe-Sb system, expressed in mol.% with SiO_2 substrate of each phase equilibrated at fixed temperature with or without preheating.

S. no.	Preheat 2 (°C/h)	Equilibration		Phase	Normalized mol. %		Unnormalized (wt.%)
		T (°C)	t (h)		Fe	Sb	
(o) BCC-Fe liquidus							
147	-	1400	5	Liquid metal	89.8 ± 0.4	10.2 ± 0.4	100.47
				BCC-Fe	98.3 ± 0.0	1.7 ± 0.0	99.72
148	-	1350	5.25	Liquid metal	86.0 ± 0.6	14.0 ± 0.6	100.40
				BCC-Fe	97.8 ± 0.0	2.2 ± 0.0	99.98
149	-	1300	3.5	Liquid metal	82.1 ± 1.2	17.9 ± 1.2	100.50
				BCC-Fe	97.3 ± 0.0	2.7 ± 0.0	99.98
150	-	1250	6.25	Liquid metal	78.7 ± 0.8	21.3 ± 0.8	100.31
				BCC-Fe	96.9 ± 0.1	3.1 ± 0.1	100.11
151	-	1200	5.5	Liquid metal	74.8 ± 0.8	25.2 ± 0.8	100.26
				BCC-Fe	96.4 ± 0.0	3.6 ± 0.0	100.17
152	-	1150	6.75	Liquid metal	72.1 ± 1.0	27.9 ± 1.0	100.36
				BCC-Fe	96.1 ± 0.0	3.9 ± 0.0	99.77
153	-	1100	3	Liquid metal	70.3 ± 0.8	29.7 ± 0.8	100.28
				BCC-Fe	95.6 ± 0.0	4.4 ± 0.0	100.21
154	-	1050	6	Liquid metal	68.3 ± 0.5	31.7 ± 0.5	100.32
				BCC-Fe	95.1 ± 0.0	4.9 ± 0.0	99.70
(p) MeX-$Fe_{1+x}Sb$ liquidus							
155	-	1020	28.75	Liquid metal	64.0 ± 0.4	36.0 ± 0.4	100.33
				MeX	59.2 ± 0.2	40.8 ± 0.2	100.16
156	-	1000	4.75	Liquid	43.8 ±	56.2 ±	100.18

				metal	0.7	0.7	
				MeX	55.1 ± 0.1	44.9 ± 0.1	100.30
157	-	975	7.5	Liquid metal	38.9 ± 1.3	61.1 ± 1.3	100.44
				MeX	54.8 ± 0.2	45.2 ± 0.2	100.21
158	-	950	26	Liquid metal	34.1 ± 1.2	65.9 ± 1.2	99.88
				MeX	54.3 ± 0.1	45.7 ± 0.1	99.93
159	1000/0.5	925	14.5	Liquid metal	30.9 ± 1.0	69.1 ± 1.0	99.94
				MeX	53.7 ± 0.1	46.3 ± 0.1	100.29
160	1000/0.5	900	20	Liquid metal	27.2 ± 1.4	72.8 ± 1.4	100.42
				MeX	53.6 ± 0.1	46.4 ± 0.1	100.11
161	1000/0.5	850	14.5	Liquid metal	21.6 ± 1.6	78.4 ± 1.6	99.83
				MeX	52.9 ± 0.2	47.1 ± 0.2	100.06
162	1000/0.5	800	15	Liquid metal	16.2 ± 0.8	83.8 ± 0.8	99.83
				MeX	52.7 ± 0.2	47.3 ± 0.2	99.72
163	1000/0.5	750	19.75	Liquid metal	11.7 ± 1.3	88.3 ± 1.3	99.67
				MeX	52.0 ± 0.2	48.0 ± 0.2	100.26
(q) MeX_2 (Me = Fe and X = Sb) liquidus							
164	1000/0.5	700	24.75	Liquid metal	5.3 ± 0.7	94.7 ± 0.0	99.77
				MeX_2	33.7 ± 0.2	66.3 ± 0.0	100.42
165	1000/0.5	650	25	Liquid metal	2.5 ± 0.2	97.5 ± 0.0	99.90
				MeX_2	33.8 ± 0.1	66.2 ± 0.0	100.36
(r) Sub-solidus							
166	1050/0.25	900	52	BCC-Fe	95.4 ± 0.0	4.6 ± 0.0	99.97
				MeX	58.4 ± 0.1	41.6 ± 0.0	99.52
167	1050/0.25	800	51	BCC-Fe	96.1 ± 0.0	3.9 ± 0.0	99.96
				MeX	56.9 ± 0.2	43.1 ± 0.0	99.85

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