REPORT

Experiment **MA-3313**, session 4

(beamline ID22; scheduled shifts – 10; start date and time: 27 October 2017 at 24:00; end date and time: 31 October 2017 at 08:00)

Russian Grant Proposal:

"Structural characterization of novel advanced materials on high-resolution synchrotron powder diffractometer ID22".

In the framework of experiment **MA-3313** in ESRF at beamline ID22, seven scientists from Moscow (Russian Federation), namely, Dr. Vladimir Chernyshev, Dr. Anna Tursina, Dr. Irina Ivanova, Dr. Elena Murashova, Dr. Andrei Ilyukhin and post-graduate students Anna Lobova and Albina Bushmeleva delivered the powder samples of 71 compounds for the measurements. The samples were loaded into quartz and borosilicate capillaries of 0.5 – 1.0 *mm* diameter. During 10 shifts (80 *h*) all the samples were measured in the 2θ ranges 0 – 15, 0 – 25, 0 – 30, 0 – 35 or 0 – 40º. Some of the compounds were measured at different temperatures from the range 80 – 673 K. In the total, 135 data sets were collected. The X-ray wavelength used was 0.450851(3) Å.

Table 1 contains the full list of the measured patterns (see Appendix).

Samples **1** – **19**, **30**, 2**3** – **34** and **78** – **88** are ternary intermetallics.
Samples **20, 21, 39** – **41** and **71** – **75** are MOFs.
Samples **35** and **36** are inorganic solid electrolites.
Samples **22**, **37** and **38** are organometallic compounds.
Samples **42** – **51** and **61** – **68** are hydrated CsY zeolites (FAU).
Samples **52** – **60**, **69** and **70** are dehydrated CsY zeolites (FAU).

All measured patterns will be used in subsequent structural analysis.

In conclusion, we estimate these 10 shifts of experimental work as extremely fruitful (as usual for ID22 high-resolution station) and thank the ID22 staff for the kind and helpful assistance.

Dr. V.V. Chernyshev
M.V.Lomonosov Moscow State University

Appendix.

Table 1. List of the patterns measured in experiment **MA-3313**, session 4.

№	User (reference) code of the sample	$2\theta_{min}$ – $2\theta_{max}$ (^{o})	Comment
	27-28 October (night)		
1	MUR-3 (*intermetallics, Murashova*)	0 – 35	RT
2	MUR-4	0 – 35	RT
3	MUR-5	0 – 35	RT
4	MUR-6	0 – 35	RT
5	MUR-7	0 – 35	RT
6	MUR-8	0 – 35	RT
7	MUR-9	0 – 35	RT
8	MUR-10	0 – 35	RT
9	MUR-11	0 – 35	RT
10	MUR-12	0 – 35	RT
11	MUR-12N	0 – 35	RT
12	TUR-15 (*intermetallics, Tursina*)	0 – 35	RT
13	TUR-16	0 – 35	RT
14	TUR-17	0 – 35	RT
15	TUR-18	0 – 35	RT
	28 October (day)		
16.1-5	MUR-1 (*High T*)	0 – 35	RT, 675, 700, 725, 750 ^{o}C
17.1-6	MUR-2 (*High T*)	0 – 35	RT, 600, 625, 650, 675, 700 ^{o}C
18	TUR-13 (*Low T*)	0 – 35	85 K
19.1-4	TUR-14 (*Low T*)	0 – 35	RT, 200, 100, 85 K
20	ISA-27 (*MOF, Isaeva*)	0 – 25	250 K
21	ISA-29 (*MOF, Isaeva*)	0 – 25	250 K
22	OK (*organic, Rybakov*)	0 – 25	250 K
	28-29 October (night)		
23	TUR-1 (*intermetallics, Tursina*)	0 – 40	RT
24	TUR-2	0 – 40	RT
25	TUR-3	0 – 40	RT
26	TUR-4	0 – 40	RT
27	TUR-5	0 – 40	RT
28	TUR-6	0 – 40	RT
29	TUR-7	0 – 40	RT
30	TUR-8	0 – 40	RT
31	TUR-9	0 – 40	RT
32	TUR-10	0 – 40	RT
33	TUR-11	0 – 40	RT
34	TUR-12	0 – 40	RT
35	TYA-1 (*inorganic, Tyablikov*)	0 – 40	RT
36	TYA-2	0 – 40	RT
	29 October (day)		
37	AB1 (*organometallic, Ilyukhin*)	0 – 25	RT
38.1-3	AB2 (*organometallic, Low T*)	0 – 25	RT, 125, 105 K
39	ISA-25 (*MOF, Isaeva*)	0 – 25	200 K
40	ISA-26	0 – 25	200 K

41	ISA-29	0 – 25	200 K
	29-30 October (night)		
42	IVA-1 (*zeolite FAU hydrated, Ivanova*)	0 – 30	RT
43	IVA-2	0 – 30	RT
44	IVA-3	0 – 30	RT
45	IVA-4	0 – 30	RT
46	IVA-5	0 – 30	RT
47	IVA-6	0 – 30	RT
48	IVA-7	0 – 30	RT
49	IVA-8	0 – 30	RT
50	IVA-9	0 – 30	RT
51	IVA-10	0 – 30	RT
52	IVK-2 (*zeolite FAU dehydrated, Ivanova*)	0 – 30	RT
53	IVK-3	0 – 30	RT
54	IVK-4	0 – 30	RT
55	IVK-5	0 – 30	RT
56	IVK-7	0 – 30	RT
57	IVK-8	0 – 30	RT
	30 October (day)		
58	IVK-1 (*zeolite FAU dehydrated, Ivanova*)	0 – 15	RT, *changed color in the beam*
59	IVK-9 (*zeolite FAU dehydrated, Ivanova*)	0 – 15	RT, *changed color in the beam*
60	IVK-1 (*Low T*)	0 – 15	200 K, *changed color in the beam*
61	IVA-1 (*Low T*)	0 – 25	200 K
62	IVA-2 (*Low T*)	0 – 25	200 K
63	IVA-4 (*Low T*)	0 – 25	200 K
64	IVA-8 (*Low T*)	0 – 25	200 K
65	IVA-1 (*High T*)	0 – 25	*High-T* = 400 C
66	IVA-2 (*High T*)	0 – 25	400 C
67	IVA-4 (*High T*)	0 – 25	400 C
68	IVA-8 (*High T*)	0 – 25	400 C
69	IVK-1 (*High T*)	0 – 25	400 C, *recovered color at heating*
70	IVK-9 (*High T*)	0 – 25	400 C, *recovered color at heating*
71	ISA-5 (*MOF, Isaeva*)	0 – 25	250 K
72	ISA-10 (*MOF, Isaeva*)	0 – 25	250 K
	30-31 October (night)		
73	ISA-11 (*MOF, Isaeva*)	0 – 25	200 K
74	ISA-12 (*MOF, Isaeva*)	0 – 25	200 K
75	ISA-14 (*MOF, Isaeva*)	0 – 25	200 K
76	IVK-1 (*zeolite FAU dehydrated, Ivanova*)	0 – 25	200 K, *changed color in the beam*
77	IVK-9 (*zeolite FAU dehydrated, Ivanova*)	0 – 25	200 K, *changed color in the beam*
	29-31 October (Gribanov)		
78.1-4	GRI-1 (*intermetallics*)	0 – 35	RT, 200, 120, 80 K
79.1-4	GRI-2	0 – 35	RT, 200, 120, 80 K
80.1-4	GRI-3	0 – 35	RT, 200, 120, 80 K
81.1-4	GRI-4	0 – 35	RT, 200, 120, 80 K
82.1-4	GRI-5	0 – 35	RT, 200, 120, 80 K
83.1-4	GRI-6	0 – 35	RT, 200, 120, 80 K
84.1-4	GRI-7	0 – 35	RT, 200, 120, 80 K
85.1-4	GRI-8	0 – 35	RT, 200, 120, 80 K

86.1-4	GRI-9	0 – 35	RT, 200, 120, 80 K
87.1-4	GRI-10	0 – 35	RT, 200, 120, 80 K
88.1-4	GRI-11	0 – 35	RT, 200, 120, 80 K