

**XRD measurements of SmS 03.11.14**

Device: BRUKER XDR D8 Advanced, Wavelength 1.54 Å, Power 1.5 kW, range  $2\theta=20-75^\circ$ , two scan regimes:

(i) "fast" 1 sec/step accumulation time and  $0.1^\circ$ /step (about 15 minutes full range)

(ii) "slow" 3 sec/step and  $0.05^\circ$ /step (about 55 minutes full range)

Results are saved as ASCII ".uxd" or ".txt" and in Bruker program format ".raw"

Samples:

KS79 annealed	Has been measured by XRD.
KS80 annealed	Has been measured by XRD.

**Basis XRD on SmS**

Open data base American Mineralogist Crystal Structure Database:

<http://rruff.geo.arizona.edu/AMS/result.php>

XPOW Copyright 1993 Bob Downs, Ranjini Swaminathan and Kurt Bartelmehs

For reference, see Downs et al. (1993) American Mineralogist 78, 1104-1107.

**SmS**

Wyckoff R W G

Crystal Structures 1 (1963) 85-237

Second edition. Interscience Publishers, New York, New York

rocksalt structure

\_database\_code\_amcsd 0011397

CELL PARAMETERS: 5.9700 5.9700 5.9700 90.000 90.000 90.000

SPACE GROUP: Fm3m

atom x y z

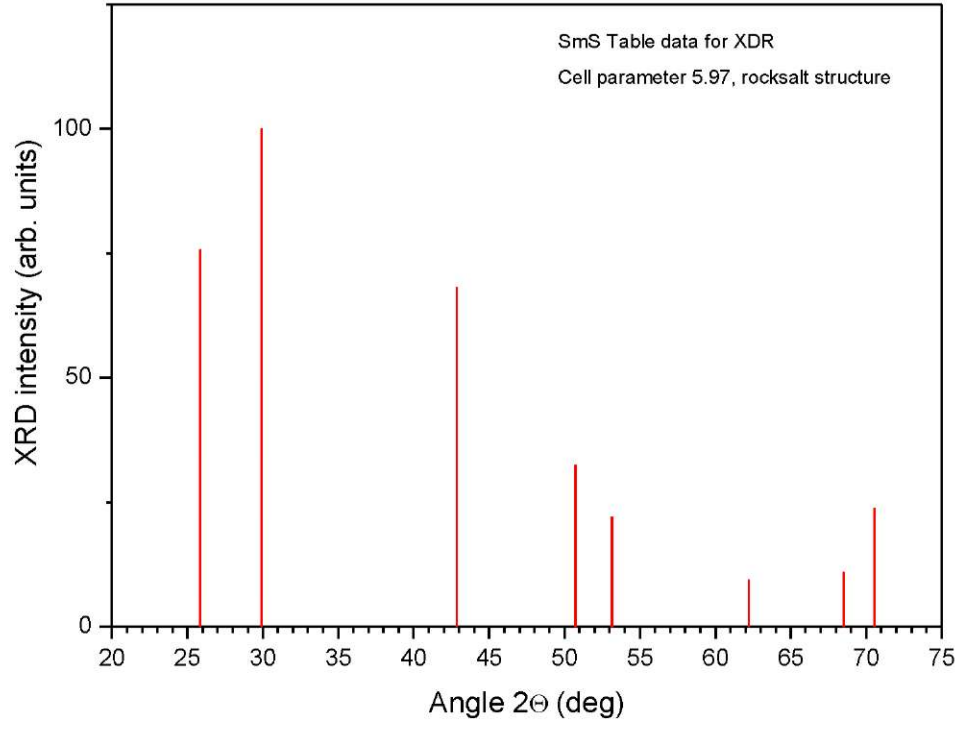
Sm 0 0 0

S .5 .5 .5

X-RAY WAVELENGTH: 1.541838

MAX. ABS. INTENSITY / VOLUME\*\*2: 225.0710623

2-THETA	INTENSITY	D-SPACING	H	K	L	Multiplicity
25.85	75.72	3.4468	1	1	1	8
29.93	100.00	2.9850	2	0	0	6
42.84	68.18	2.1107	2	2	0	12
50.72	32.44	1.8000	3	1	1	24
53.14	21.94	1.7234	2	2	2	8
62.20	9.37	1.4925	4	0	0	6
68.51	10.93	1.3696	3	3	1	24
70.55	23.80	1.3349	4	2	0	24
78.49	16.47	1.2186	4	2	2	24
84.29	5.26	1.1489	5	1	1	24
84.29	1.75	1.1489	3	3	3	8

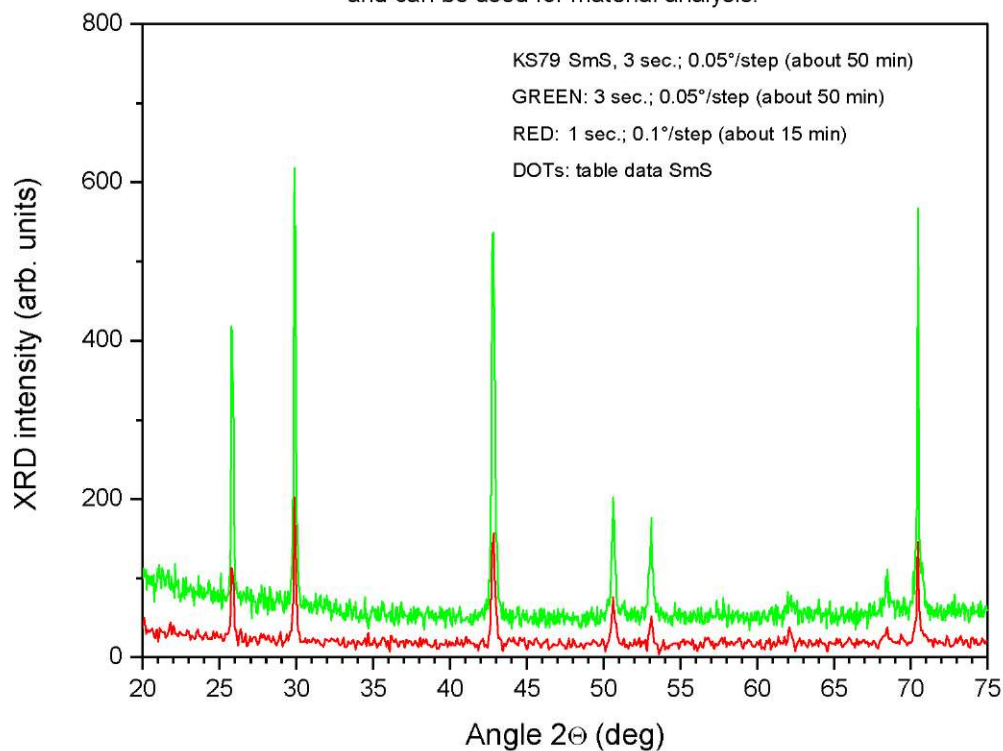


## Experimental Results

### KS79 annealed

Bruker D8, 1.5 kW, 1.54 Angstrom

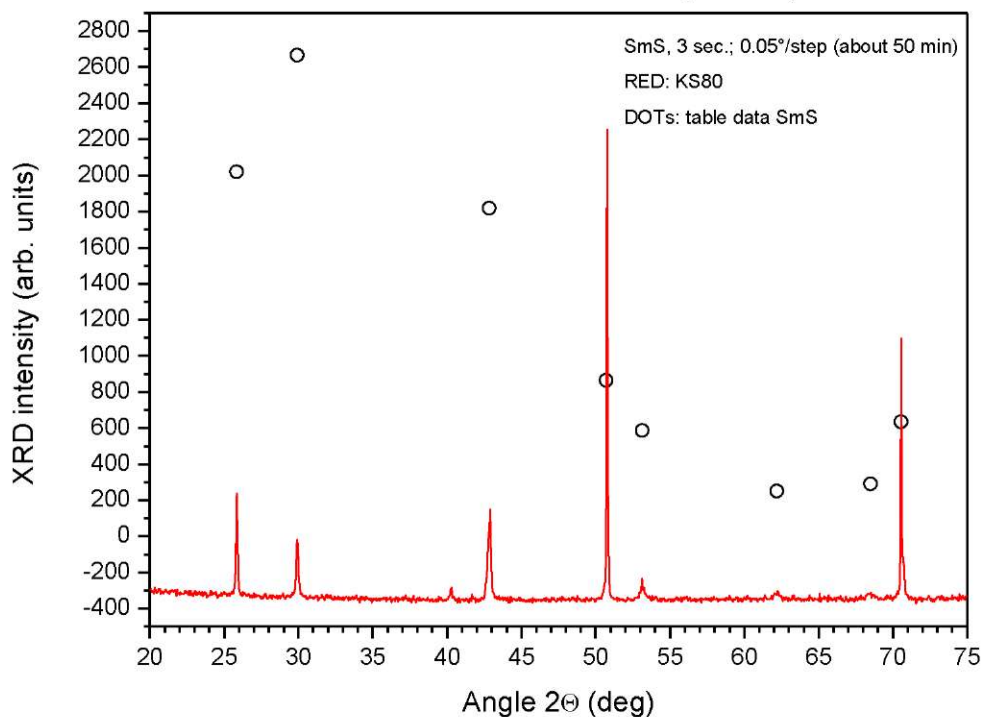
Conclusion: already 15 min run shows most of features and can be used for material analysis.



### KS80 annealed

Bruker D8, 1.5 kW, 1.54 Angstrom

Conclusion: ALL peaks correspond to table data for SmS, while relative intensities between peaks vary.



## Comparison KS79 and KS80

Bruker D8, 1.5 kW, 1.54 Angstrom

Conclusion: ALL peaks correspond to table data for SmS, while relative intensities between peaks vary.

