MECHANOCHEMICAL SYNTHESIS AS A TOOL FOR MODELING PROPERTIES OF (NEW?) IRON CARBIDES

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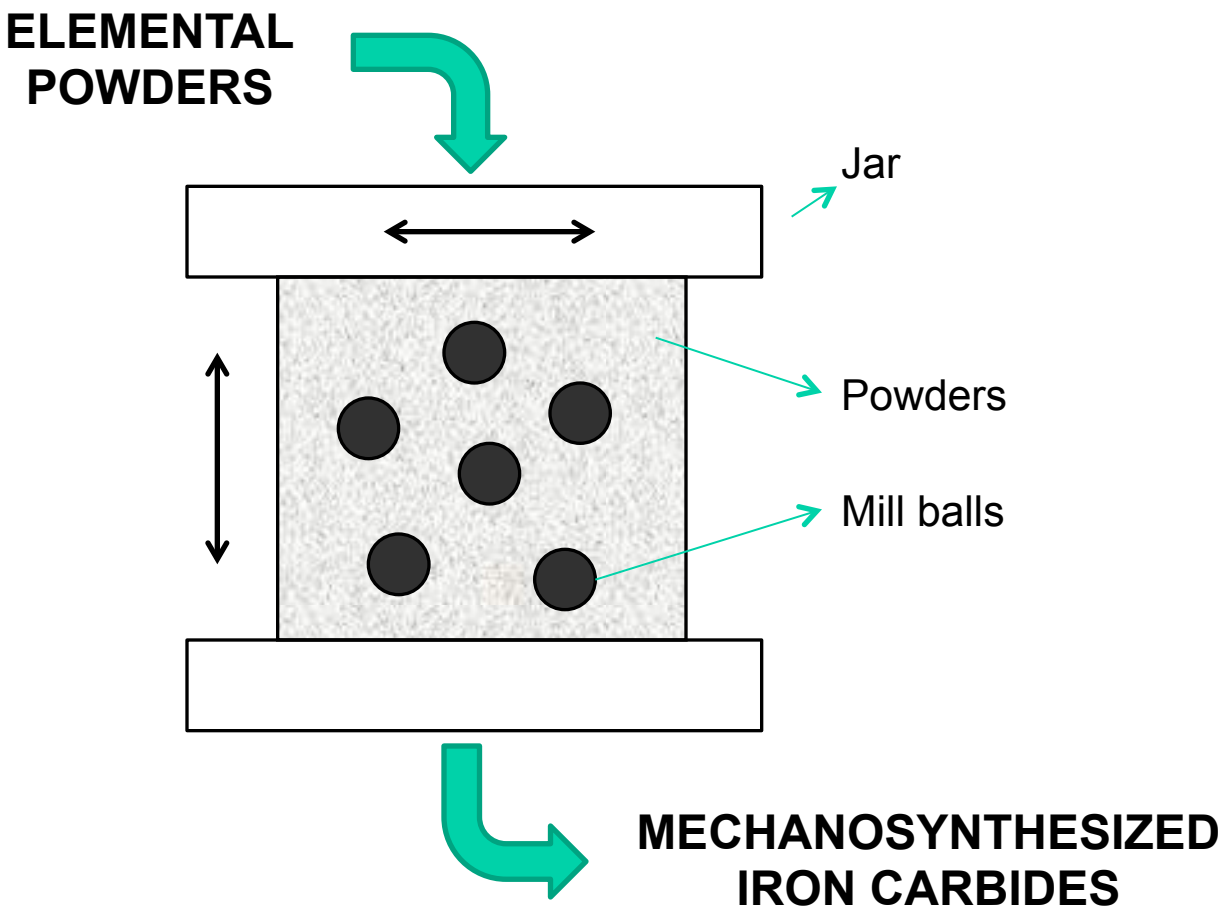
A.D. MDLXII
UNIVERSITÀ DEGLI STUDI DI SASSARI

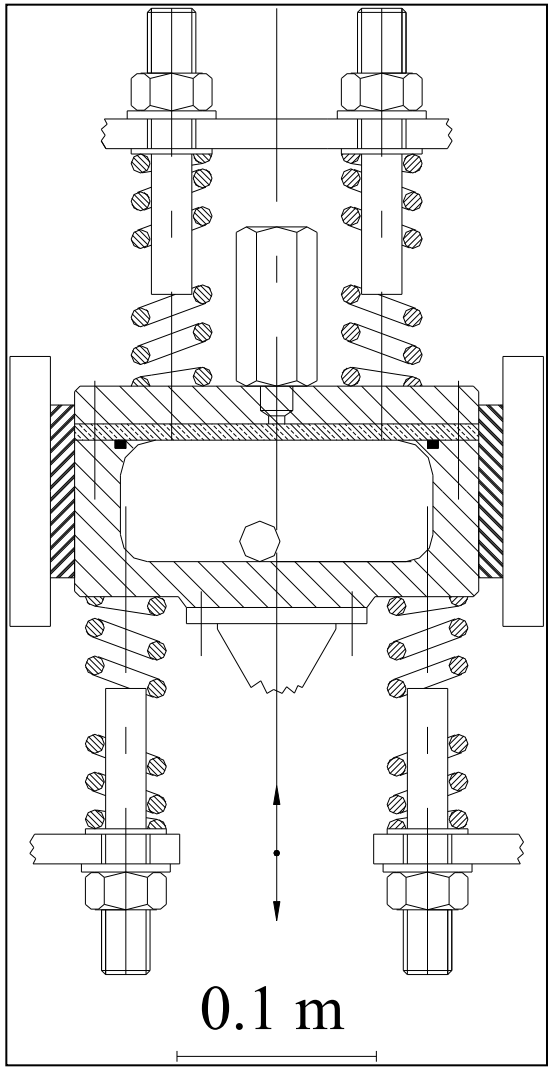
SUMMARY

1. Principles of mechanosynthesis of iron carbides
2. Characterization by means of Mossbauer spectroscopy
3. Kinetic approach to mechanochemical synthesis
4. Remarks on recent results on the formation of iron carbides and their thermal stability
5. Conclusions

MECHANOSYNTHESIS OF IRON CARBIDES

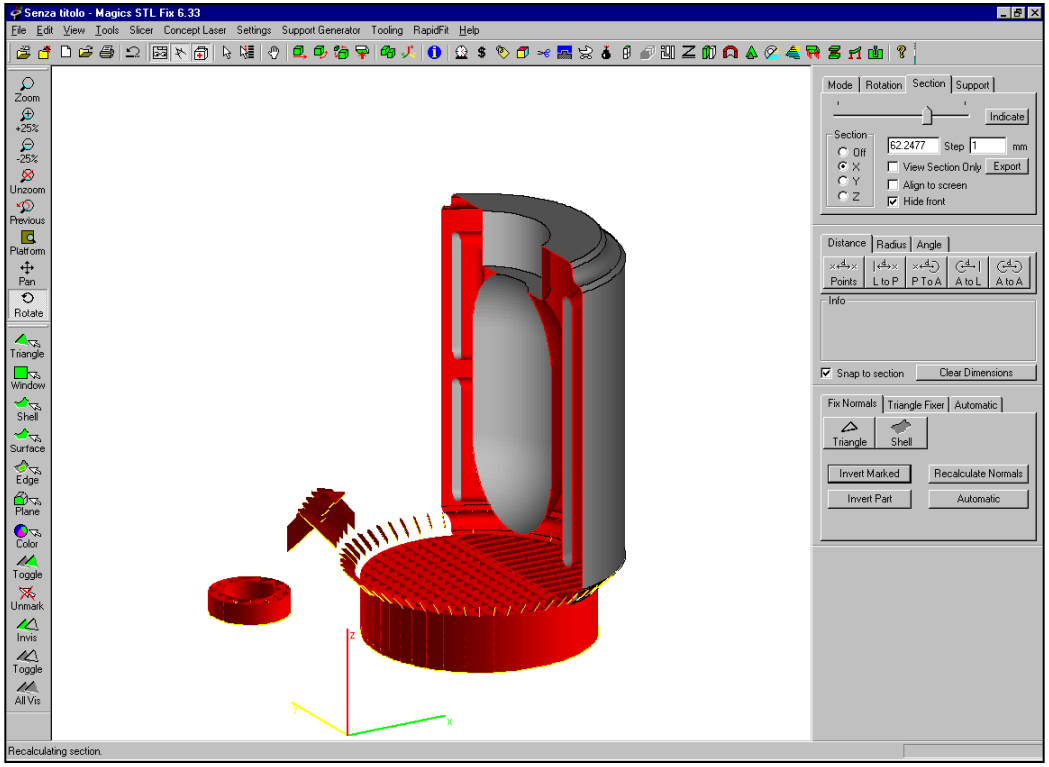


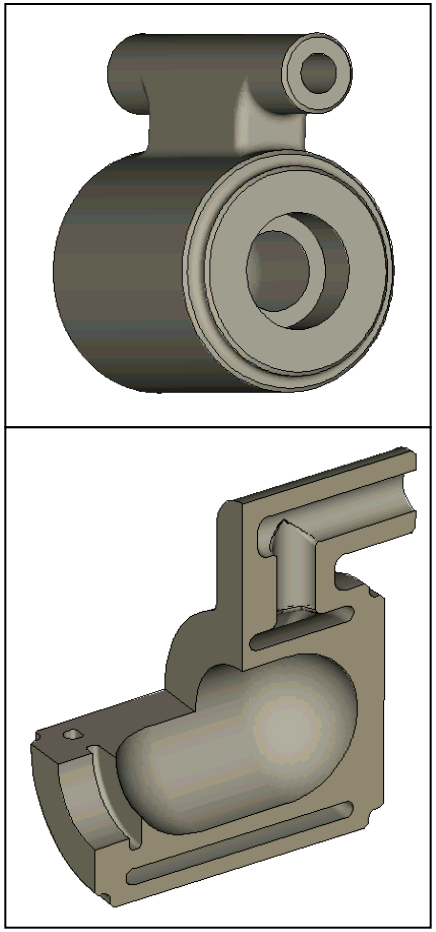
EXPERIMENTAL MILL



Vibrating mill for mechanosynthesis of iron carbides

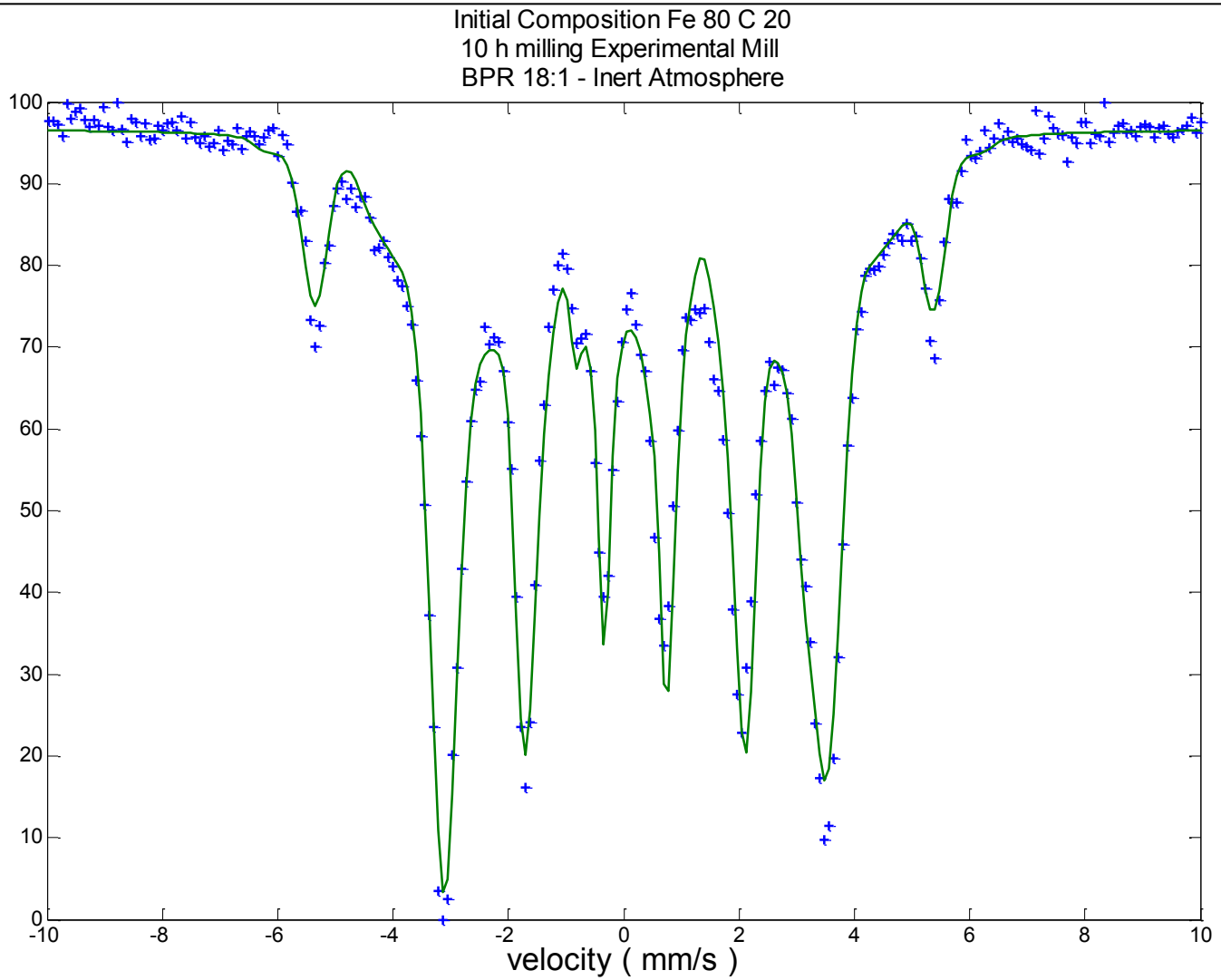
PROTOTYPE VIAL



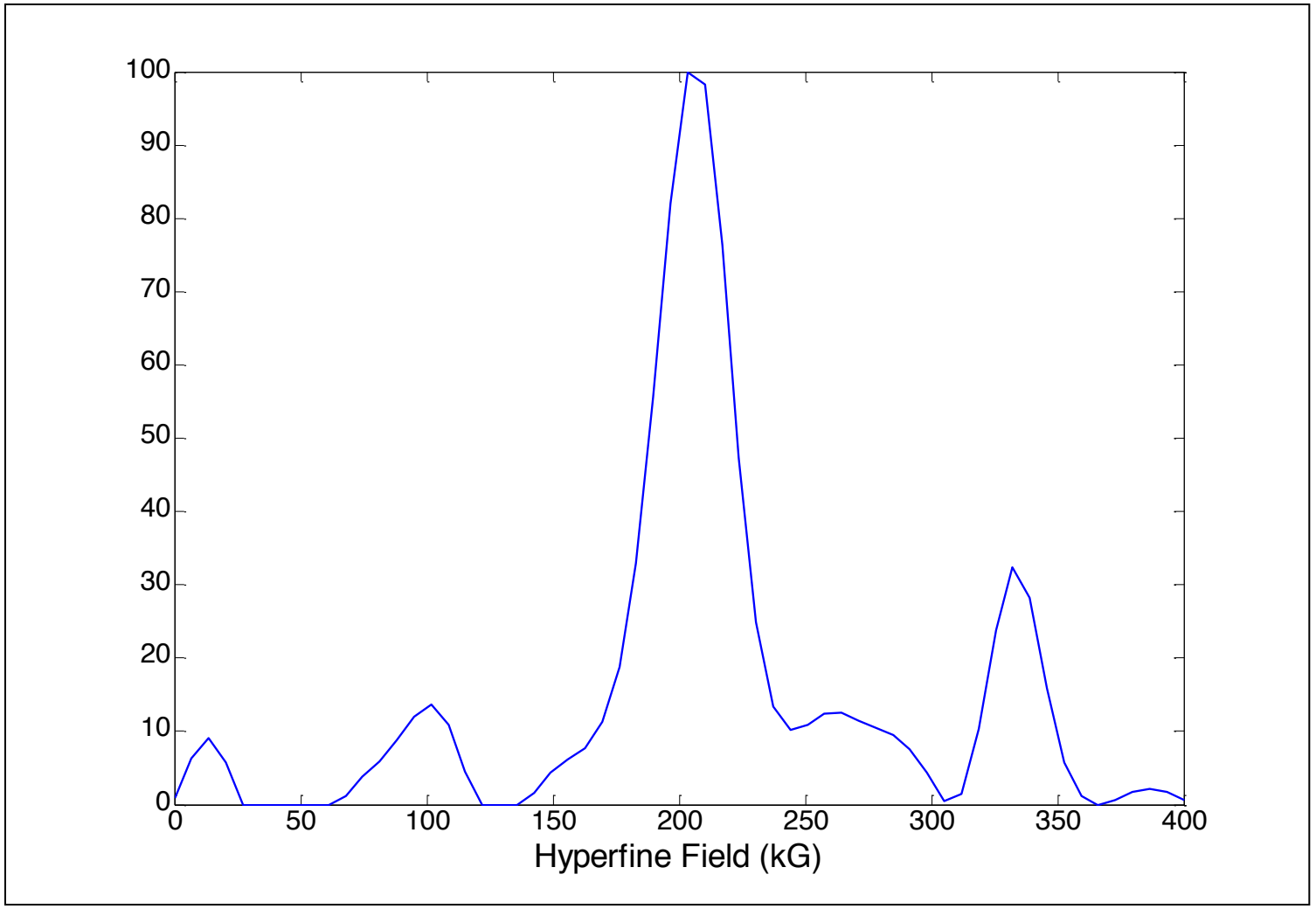


Prototype vial for the Spex 8000Mill, constructional details along with a sectioned view of internal channels.

MOESSBAUER SPECTROSCOPY



MOESSBAUER SPECTROSCOPY: Hyperfine Field Distribution



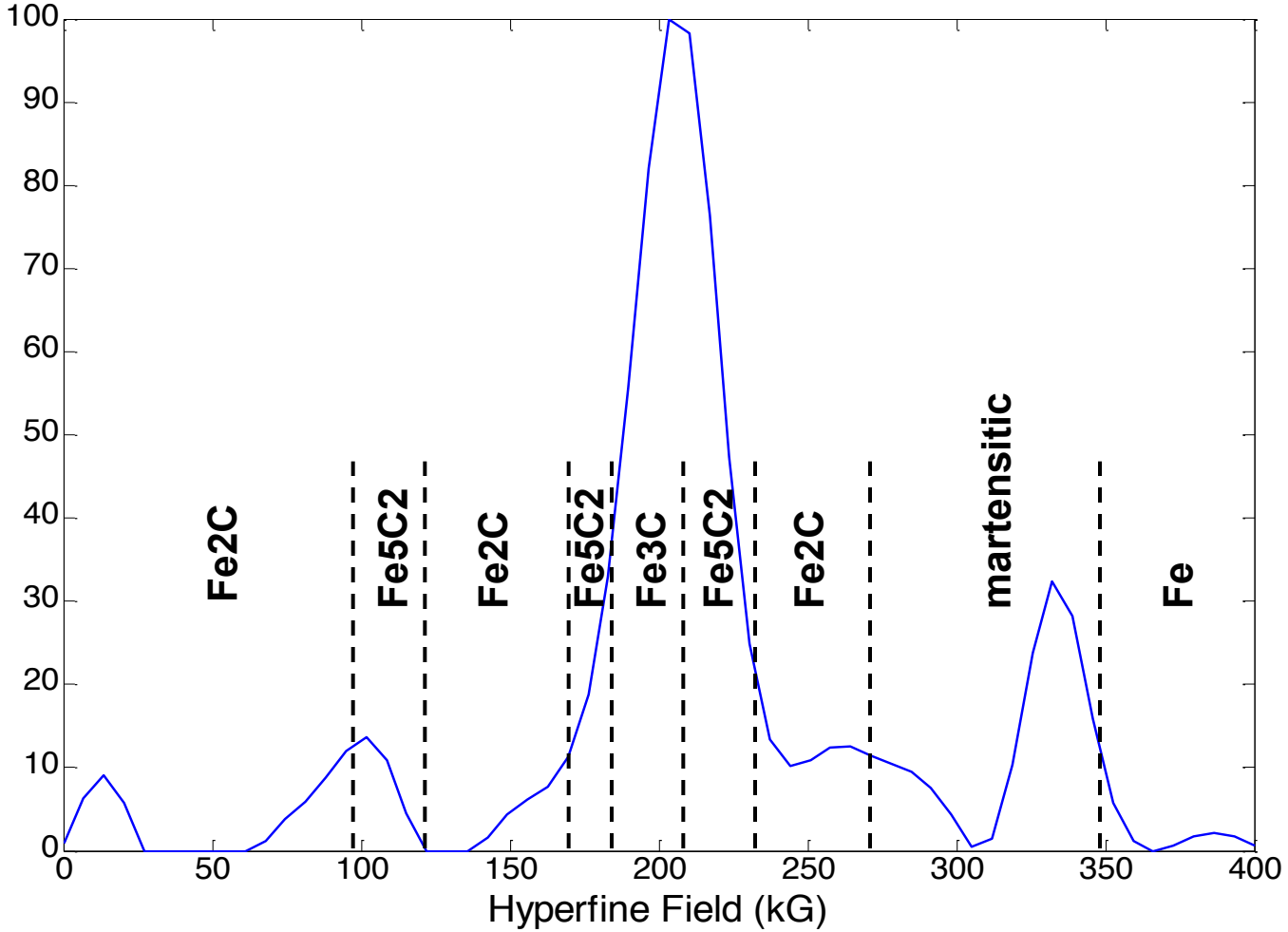
TECHNICAL details: Hyperfine Field Distribution Assignment

	Field, kG		
Fe	300-350		
Fe3C	185-215		
Fe2C	0-95	130-170	230-270
Fe5C2	95-130	170-185	215-230
“Martensitic”	270-300		
Fe7C3	-	In progress..	

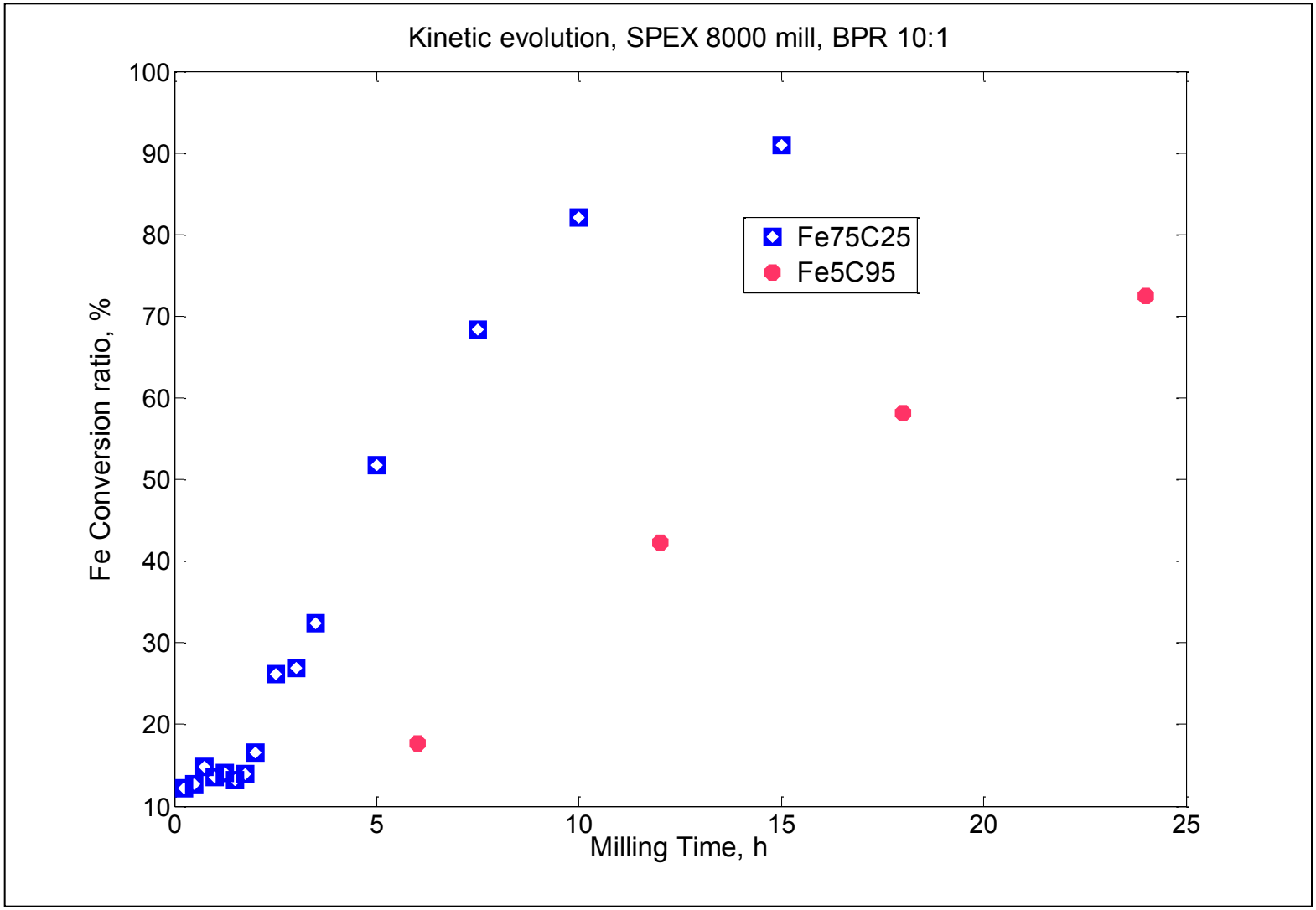
TECHNICAL details: Hyperfine Field Distribution Assignment

Field, kG		Isomer Shift (mm/s)
0-95	Fe2C	0.03
95-130	Fe5C2	0.02
130-170	Fe2C	0.02
170-185	Fe5C2	0.02
185-215	Fe3C	0.02
215-230	Fe5C2	0.02
230-270	Fe2C	0.02
270-300	“Martensitic”	0
300-350	Fe	0

CALCULATION OF PHASE FRACTION



KINETIC APPROACH



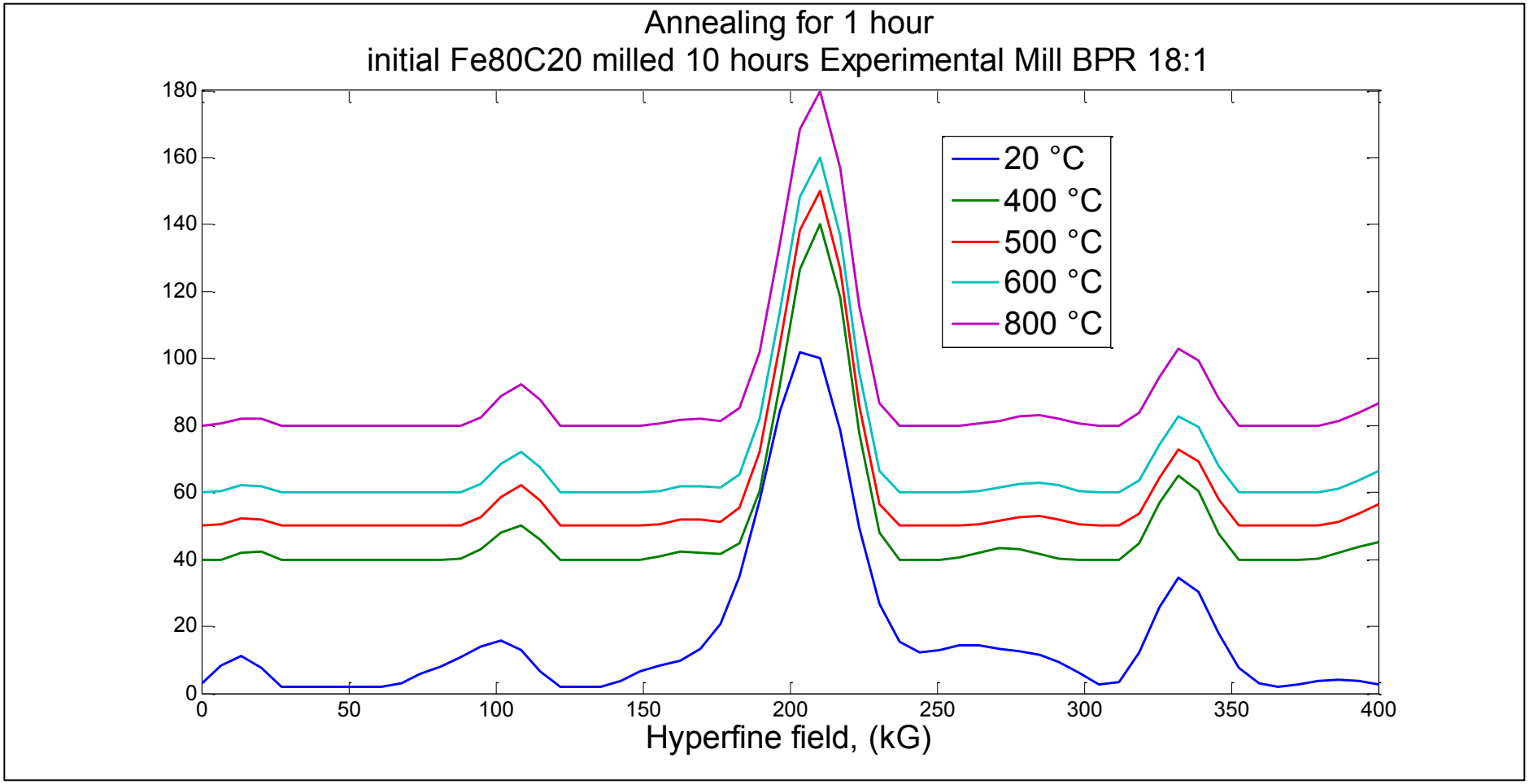
KINETIC RESULTS Fe5C95 BPR 10:1, Spex 8000 Mill

milling time, h	Fe	Fe2C	Fe5C2	Fe3C	Martens
6	82,4	7,0	3,5	6,8	0,5
12	57,7	17,2	7,6	16,6	0,9
18	41,8	25,3	9,7	22,4	0,8
24	27,5	31,8	13,3	25,7	1,6

KINETIC RESULTS Fe75C25 BPR 10:1, Spex 8000 Mill

milling time, h	Fe	Fe2C	Fe5C2	Fe3C	Martens
0,25	87,8	3,8	3,4	4,9	0,0
0,5	87,3	3,7	3,7	5,3	0,0
0,75	85,2	4,0	3,8	6,7	0,3
1	86,4	5,5	3,4	4,6	0,1
1,25	85,9	5,6	3,5	4,8	0,2
1,5	86,8	6,6	2,6	2,4	1,6
1,75	86,1	7,2	2,7	3,5	0,5
2	83,4	8,3	2,8	4,6	0,9
2,5	73,8	11,0	5,0	8,0	2,2
3	73,1	12,3	5,4	7,2	1,9
3,5	67,6	13,6	7,6	8,2	3,0
5	48,2	17,7	11,5	17,9	4,8
7,5	31,6	21,2	16,0	24,4	7,0
10	17,9	23,9	20,5	31,0	6,7
15	9,0	30,4	23,1	31,0	6,6

IRON CARBIDES THERMAL STABILITY



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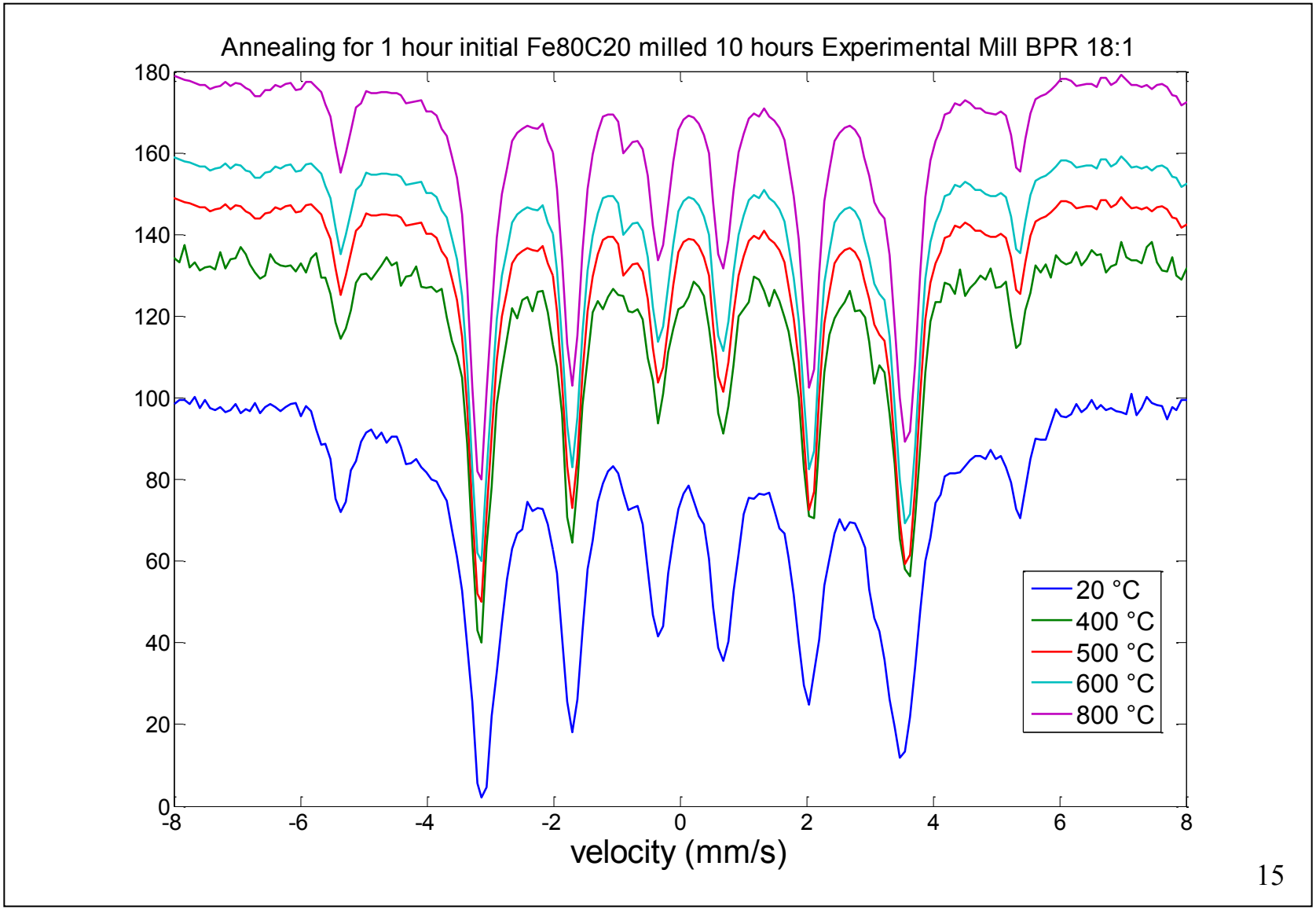

ANNEALING FOR 1h Fe80C20 MILLED FOR 10 h, BPR 18:1, Experimental Mill

annealing temperature, °C	Fe	Fe2C	Fe5C2	Fe3C
25	14,1	17,3	18,4	46,9
25	13,8	17,6	17,8	47,6
400	15,0	5,0	13,7	65,4
465	15,4	5,2	11,5	66,9
500	26,9	1,1	10,2	61,6
580	20,2	1,9	9,9	66,7
700	13,4	2,6	15,2	67,1
825	35,0	2,1	7,6	55,3

CONCLUSIONS

- Mechanochemical synthesis (mechanosynthesis) of different iron carbides is feasible and interesting for the many different carbides that may be synthesized with a simple experimental technique
- We have synthesized Fe3C, different Fe2C carbides and Fe5C2
- We are now working towards understanding thermal stability
- The whole topic might be useful for:
  - fundamental studies for properties of steels
  - providing "non-equilibrium" materials data for Calphad method modeling
  - (outside this conference..) provide iron carbides as catalysts for heterogeneous catalysis
  - (outside this conference..) provide materials that are currently considered to be components of the earth's inner core