

Electronic Supplementary Information (ESI)

Kinematic modelisation and parametric study of mechanosynthesis of hydroxyfluorapatite

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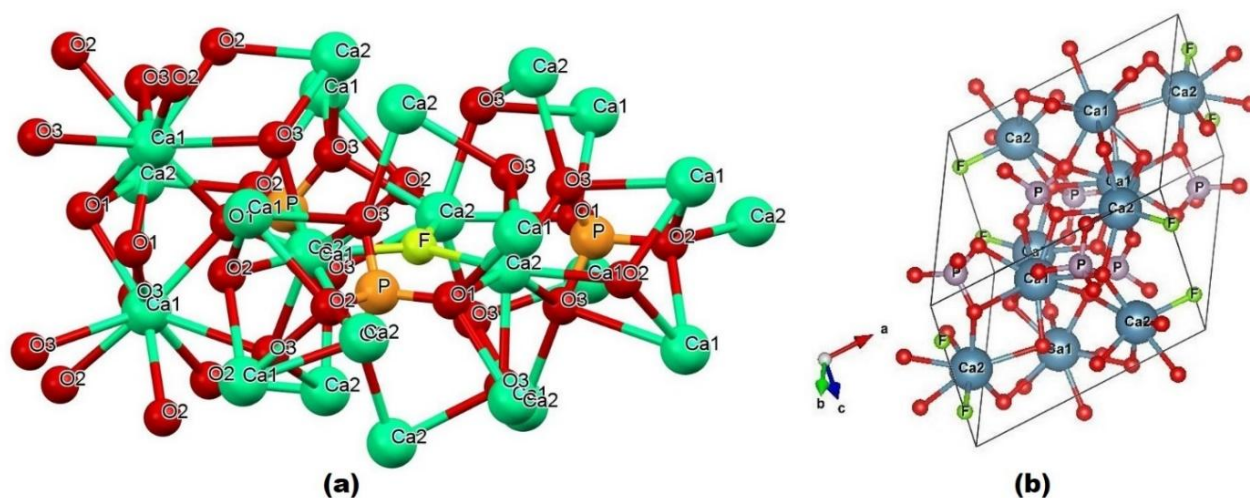
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Table S1: Injected power values for different disc rotation speed values

Disc rotation speed Ω (rpm)	P_{inj} (Nb=1, mp=1g) (w/g)
150	0.0615
250	0.2851
350	0.7824
450	1.6630

Table S2: Injected power values as a function of Nb and mp with constant disc rotation speed

450rpm					
mp (g)	P_{inj} (Nb=1) (w/g)	P_{inj} (Nb=3) (w/g)	P_{inj} (Nb=5) (w/g)	P_{inj} (Nb=6) (w/g)	P_{inj} (Nb=7) (w/g)
1.0	1.6631	4.989	8.315	9.978	11.641
1.2	1.3858	4.157	6.929	8.3148	9.7006
1.4	1.1878	3.563	5.939	7.1268	8.3146
1.7	0.9782	2.935	4.891	5.8692	6.8474

**Fig. S1:** Representation of the crystalline structure of hydroxyfluorapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})\text{F}$ (space group $\text{P6}_3 / \text{m}[1]$): (a) Mercury graph (b) Vesta graph.

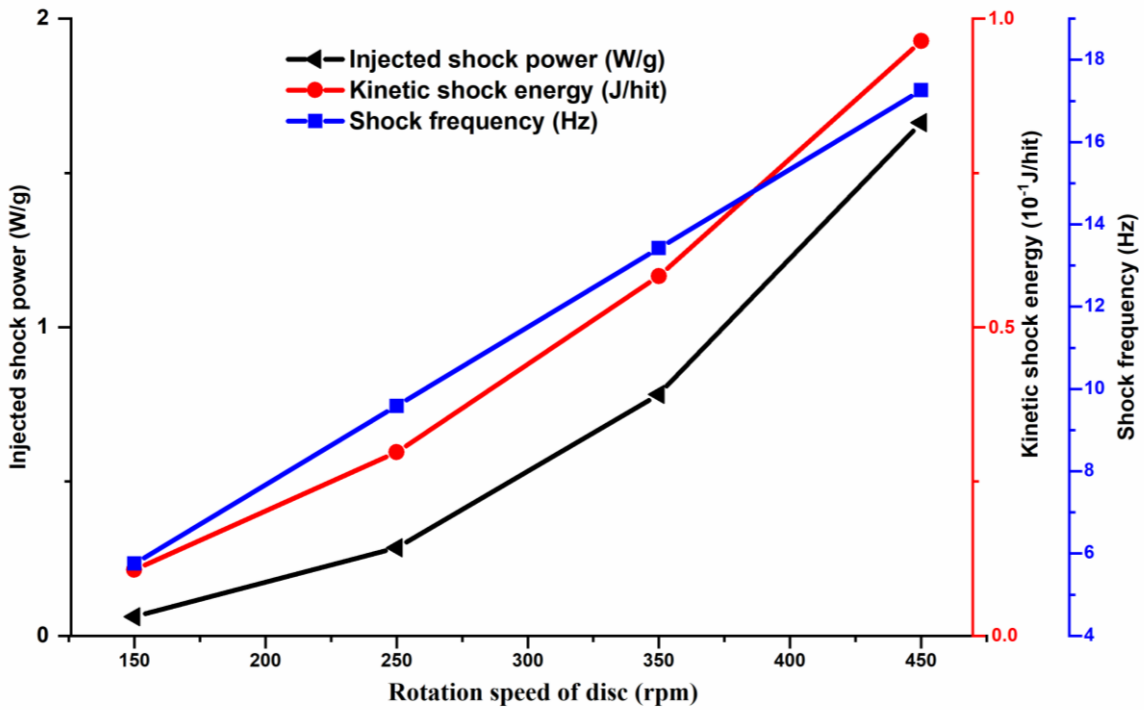


Fig.S2: Variation of the injected shock power (P_{inj}), shock frequency (F_{shoc}) and kinetic shock energy (E_{cc}) as a function of the disc rotation speed ($m_p = 1\text{ g}$, $N_b = 1\text{ ball}$)

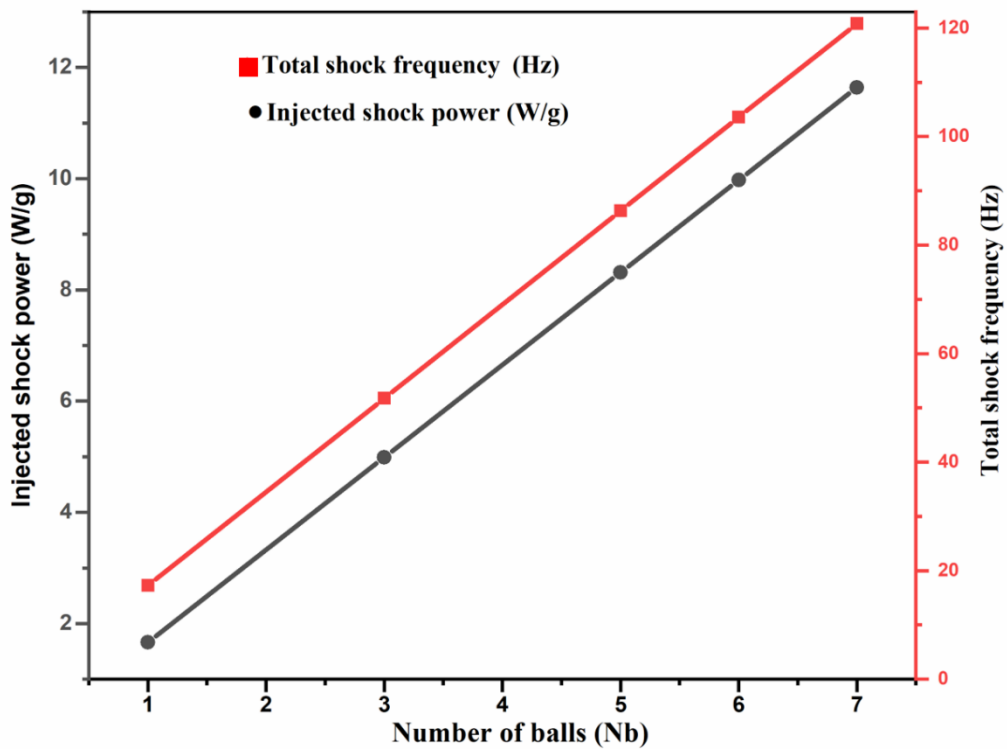


Fig. S3: Variation of the injected shock power (P_{inj}) and the total shock frequency (F_{choc}) as a function of the number of balls ($m_p = 1\text{ g}$, $\Omega = 450\text{ rpm}$)

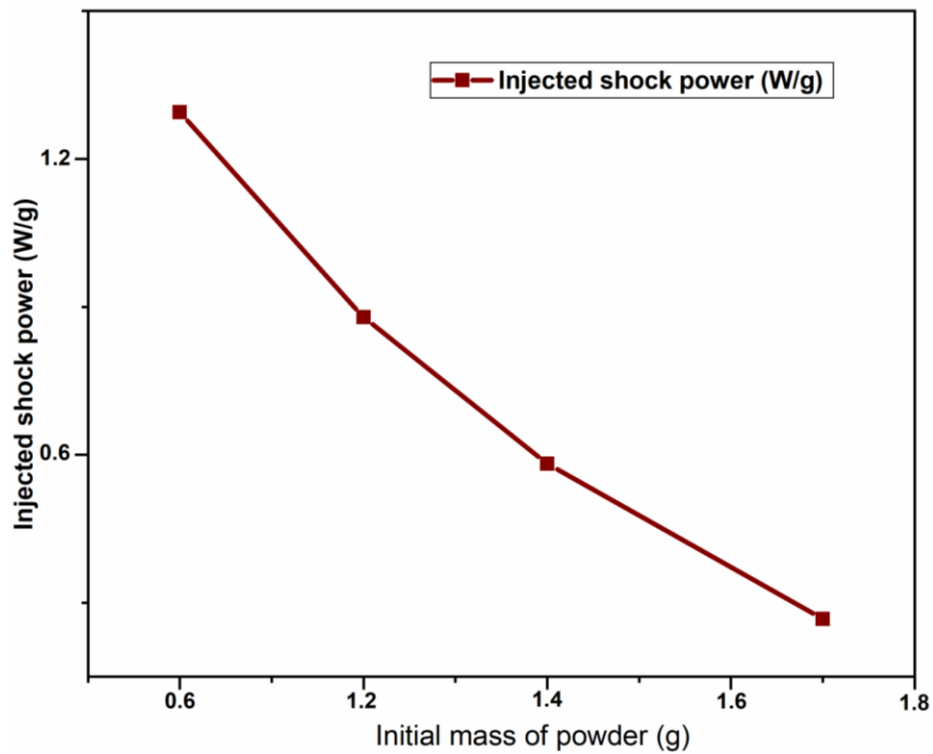


Fig.S4: Injected shock power (P_{inj}) as a function of powder mass ($N_b = 1, \Omega = 450$ rpm)

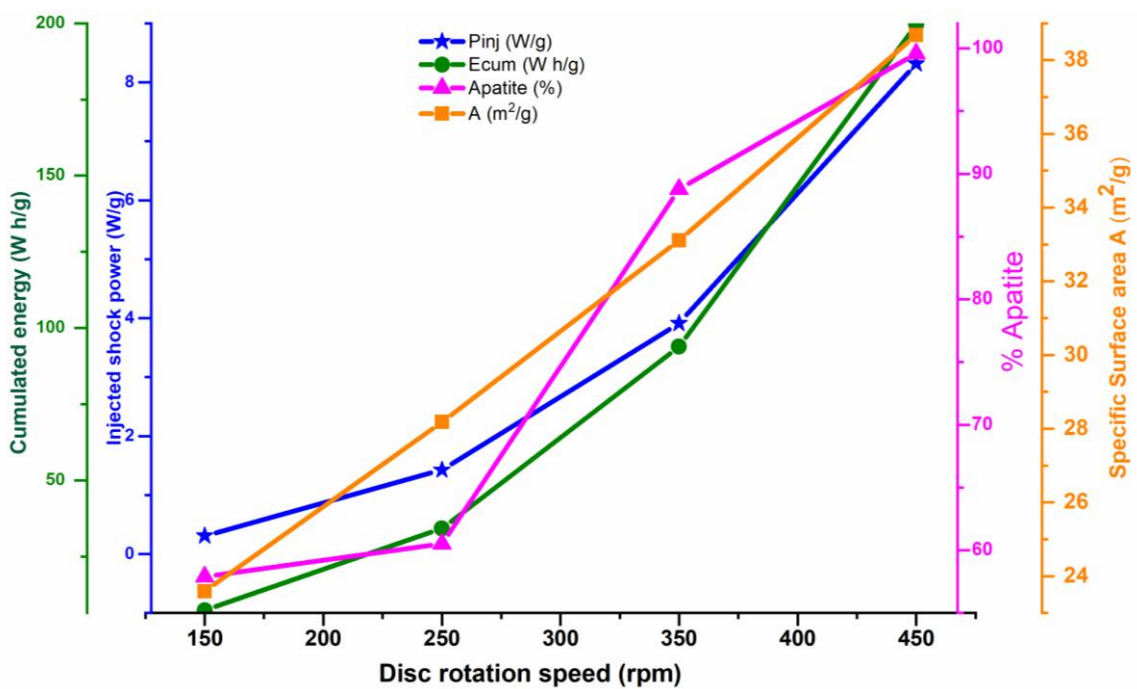


Fig. S5: Variation of the apatite content, the injected shock power (P_{inj}), the cumulated energy (E_{cum}) and the **specific surface** area (A) as a function of the disc rotation speed ($m_p = 1.2g, 6$ balls and 24 h).

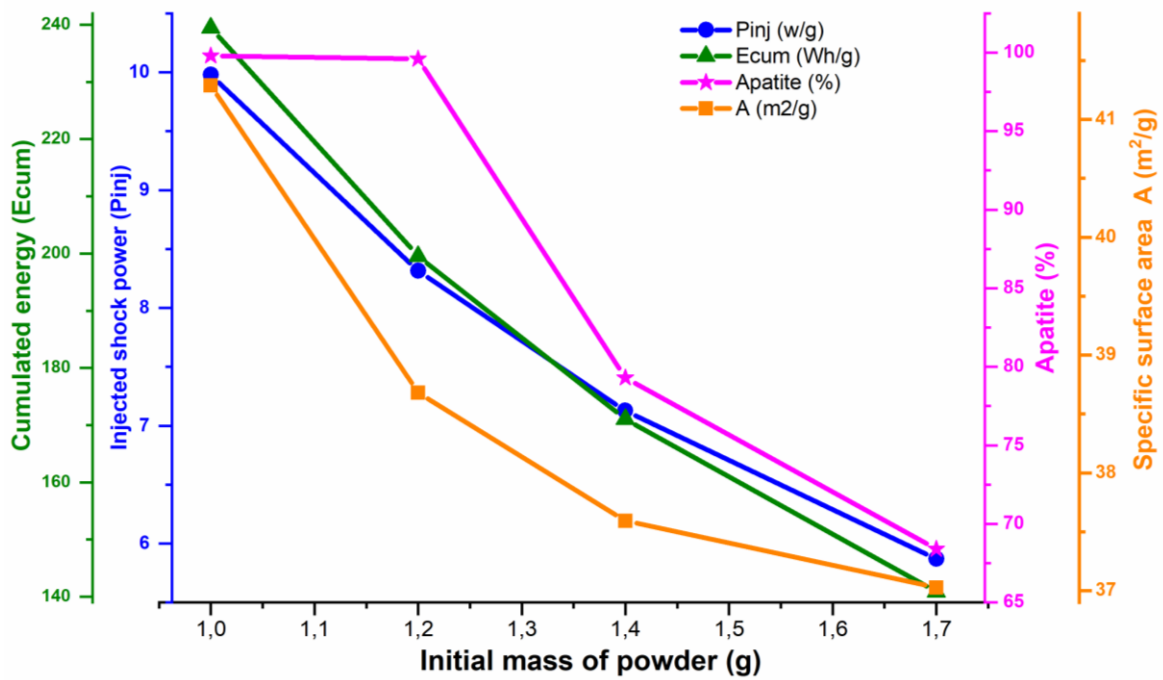


Fig. S6: Variation of the apatite content, the injected shock power (P_{inj}), the cumulated energy (E_{cum}) and the specific surface area (A) as a function of the initial mass of powder ($\Omega= 450$ rpm, 6 balls and 24 h).

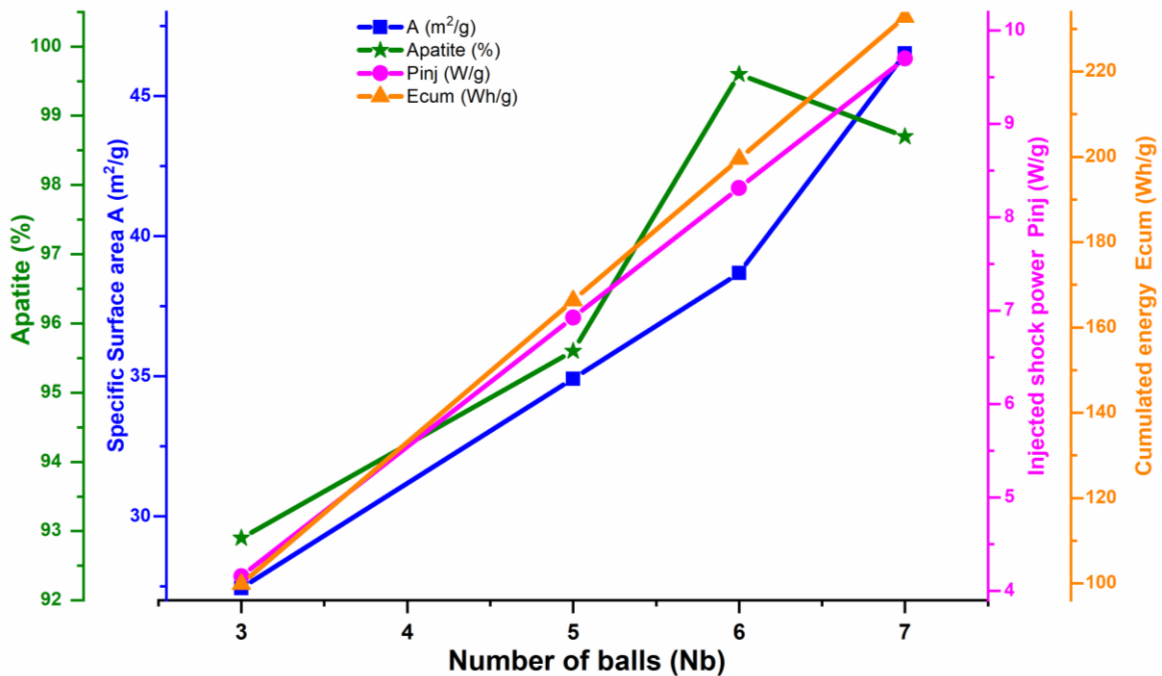


Fig. S7: Variation of the apatite content, the injected shock power (P_{inj}), the cumulated energy (E_{cum}) and the specific surface area (A) as a function of the number of balls ($\Omega= 450$ rpm, $m_p= 1.2$ g and 24 h).

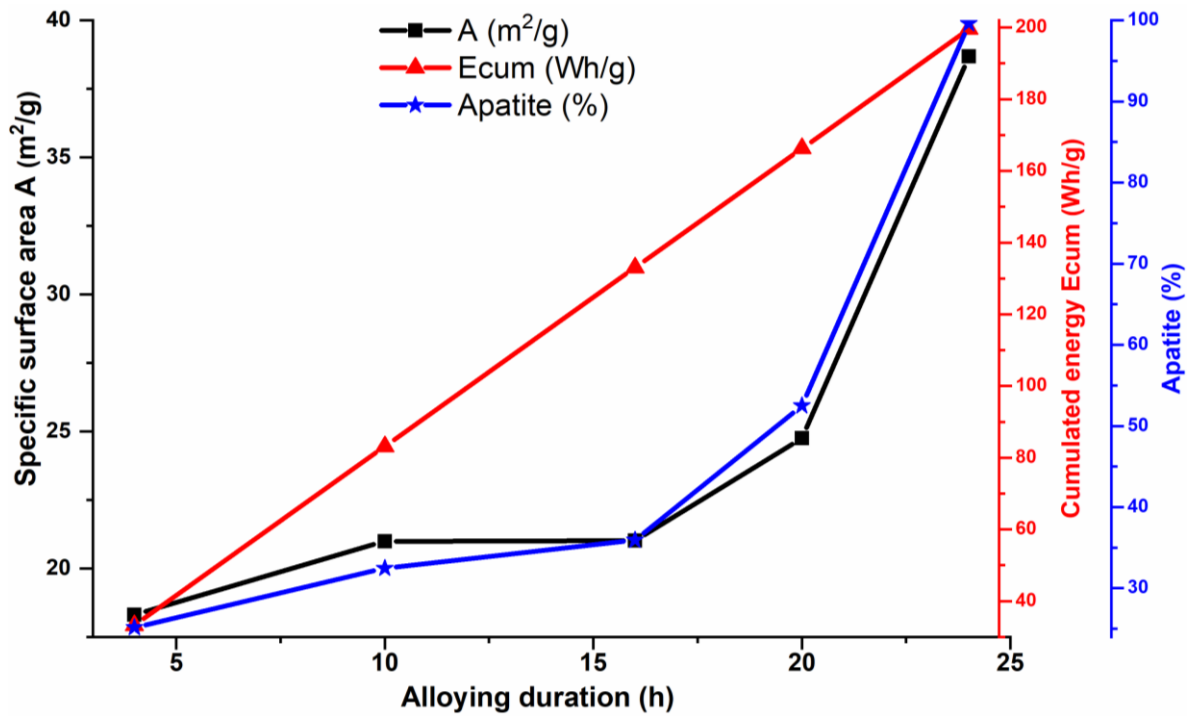


Fig. S8: Variation of the apatite content, the cumulated energy (E_{cum}) and the specific surface area (A) as a function of the grinding duration ($\Omega= 450$ rpm, $m_p= 1.2$ g, $N_b=6$, $P_{inj}=8.315$ Wh/g).

Table S3: Atomic concentration, determined by XPS and EDS analysis, of the different chemical elements in the HFA sample synthesized with the optimal conditions.

Chemical element	C1s	O1s	F1s	P2p	Ca2p	Fe2p	Ca/P
Atomic concentration (at. %) (XPS)	3.6	61.1	2.7	13.2	19.2	0.2	1.457
Atomic concentration (at. %) (EDS)	-	61.7	3.8	14.1	20.5	-	1.454

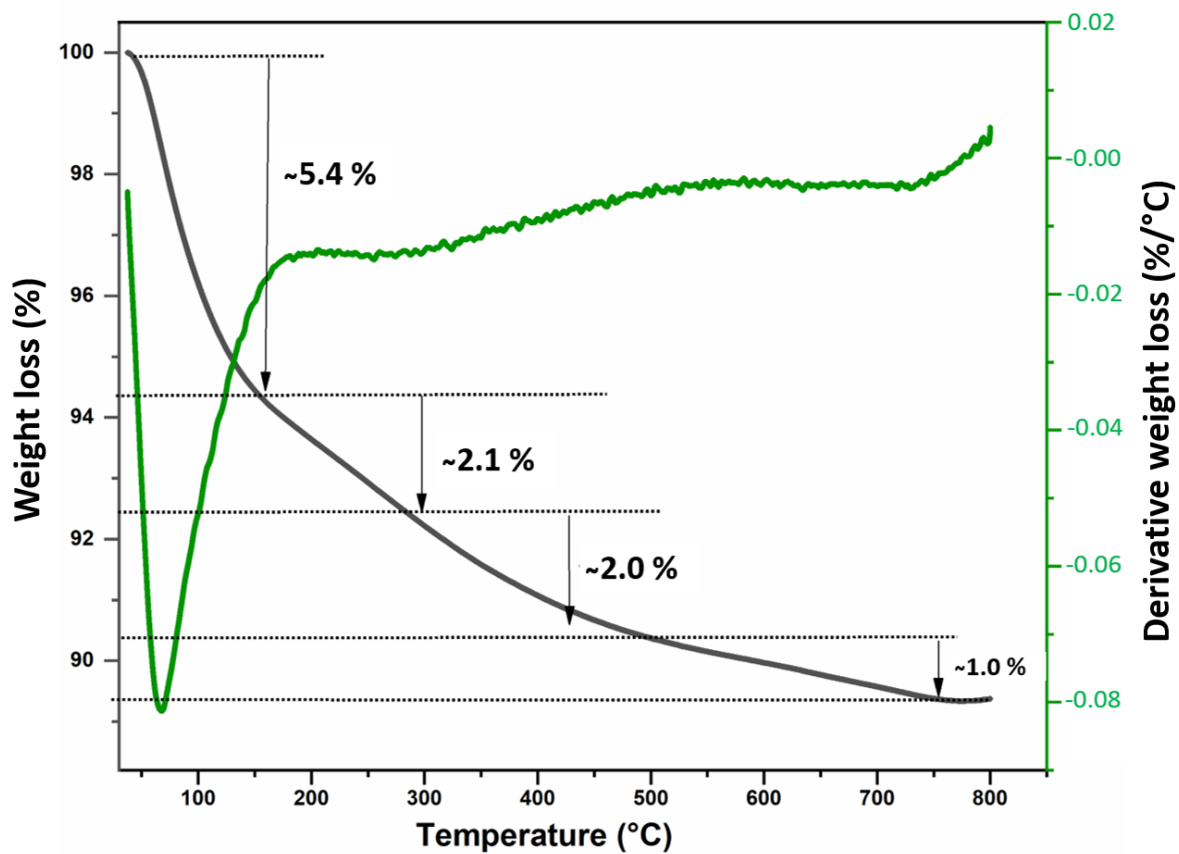


Fig. S9: Thermogravimetric analysis curves of the HFA sample synthesized with the optimal milling conditions (450 rpm, 1.2g, 6 balls and 24h).

References

- [1] Y. Gao, N. Karpukhina, et R. V. Law, Phase segregation in hydroxyfluorapatite solid solution at high temperatures studied by combined XRD/solid state NMR, *RSC Adv.* 6 (105) (2016) 103782- 103790. <https://doi.org/10.1039/C6RA17161C>.