

# Impact of rare earth elements on CaCO<sub>3</sub> crystallisation: Insights into kinetics, mechanisms, and crystal morphology

Luca Terribili<sup>1\*</sup>, Remi Rateau<sup>1</sup>, Adrienn M. Szucs<sup>1</sup>, Melanie Maddin<sup>1</sup>, Juan Diego Rodriguez-Blanco<sup>1\*</sup>.

\* [terribil@tcd.ie](mailto:terribil@tcd.ie), [J.D.Rodriguez-Blanco@tcd.ie](mailto:J.D.Rodriguez-Blanco@tcd.ie)

<sup>1</sup> Department of Geology. School of Natural Sciences. Trinity College Dublin, D02 PN40, Ireland

## SUPPORTING INFORMATION FOR THE PAPER

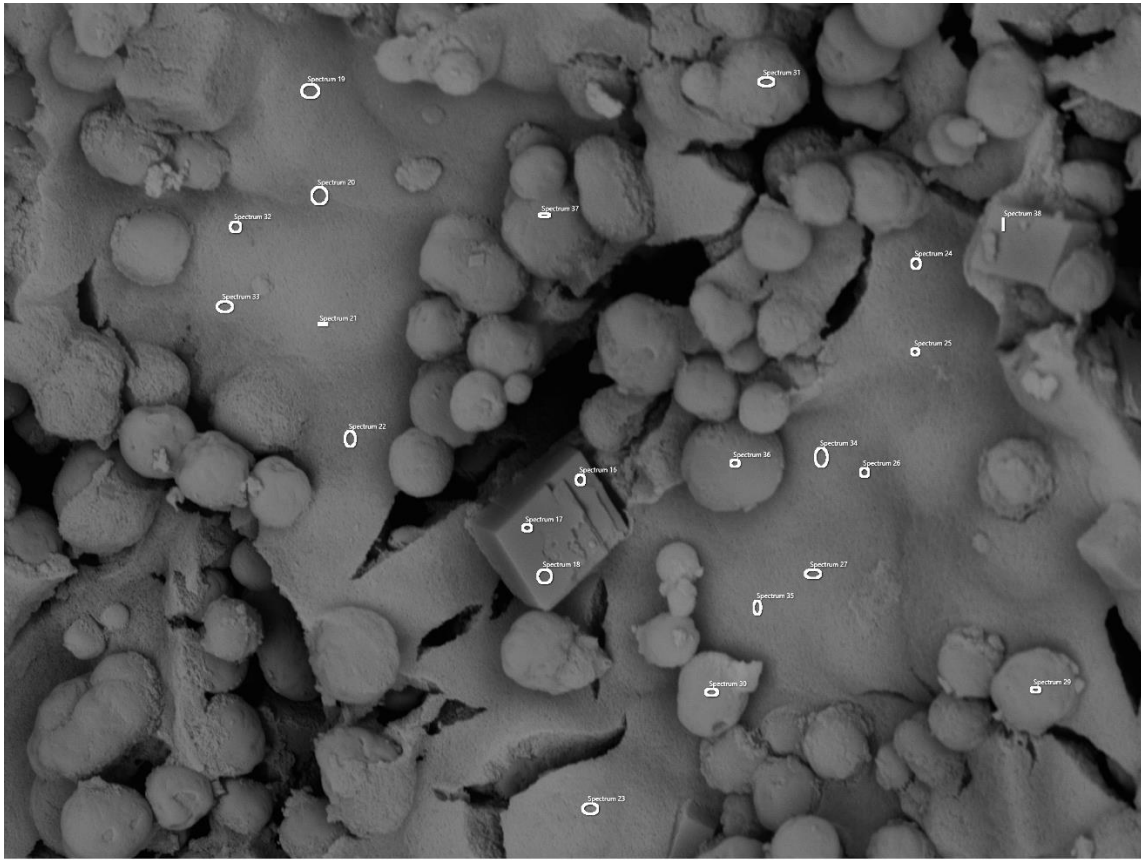
**Table SI-1.** Quantification values of the wt% of crystalline phases carried out with the Rietveld refinement software TOPAS. The values displayed refer to the Pure system (0 mM of REEs) as well to the lower and higher concentration experiments for every REE and combination of REEs used.

REE	Concentration	Calcite	Vaterite
<b>Pure System</b>	0 mM	95%	5%
<b>La</b>	0.06 mM	60%	40%
<b>La</b>	0.3 mM	31%	69%
<b>Nd</b>	0.06 mM	68%	32%
<b>Nd</b>	0.3 mM	64%	36%
<b>Dy</b>	0.06 mM	64%	36%
<b>Dy</b>	0.3 mM	39%	61%
<b>LaNd</b>	0.06 mM	46%	54%
<b>LaNd</b>	0.3 mM	62%	38%
<b>LaDy</b>	0.06 mM	40%	60%
<b>LaDy</b>	0.3 mM	42%	58%
<b>NdDy</b>	0.06 mM	52%	48%
<b>NdDy</b>	0.3 mM	72%	28%
<b>LaNdDy</b>	0.06 mM	31%	69%
<b>LaNdDy</b>	0.3 mM	32%	68%

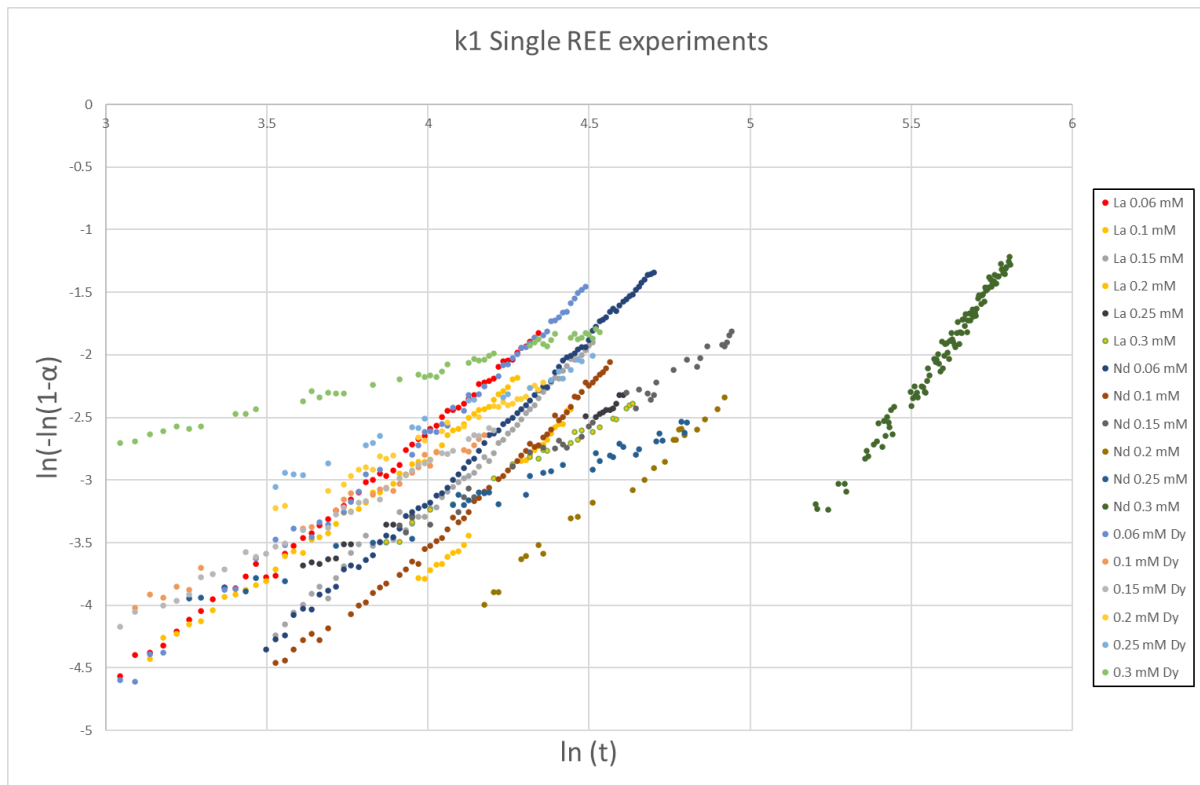
**Table SI-2.** Points of analysis obtained both on CaCO<sub>3</sub> polymorphs (calcite and vaterite) and on a homogeneous amorphous Nd- and Ca-bearing phase in an experiment with 0.3 mM of Nd. In Fig SI-1 is showed the exact location where the points of analysis were carried out.

Point of analysis	Atomic %		
	Oxygen	Calcium	Neodymium
Spectrum 16	79.22	19.57	1.21
Spectrum 17	81.15	18.50	0.35
Spectrum 18	78.24	20.94	0.81
Spectrum 19	68.39	21.85	9.76
Spectrum 20	68.64	17.90	13.45
Spectrum 21	77.19	15.55	7.26
Spectrum 22	66.75	24.90	8.35
Spectrum 23	83.53	14.31	2.18
Spectrum 24	71.14	21.91	6.95
Spectrum 25	72.86	17.54	9.60
Spectrum 26	60.08	22.19	17.73
Spectrum 27	58.34	24.54	17.12
Spectrum 29	84.40	14.78	0.82
Spectrum 30	81.00	17.67	1.33
Spectrum 31	84.83	14.46	0.71
Spectrum 32	62.13	23.71	14.16
Spectrum 33	71.79	17.20	10.99
Spectrum 34	67.16	17.47	15.39
Spectrum 35	62.34	22.71	14.95
Spectrum 36	79.86	19.01	1.13
Spectrum 37	80.29	18.82	0.87
Spectrum 38	84.91	13.73	1.36

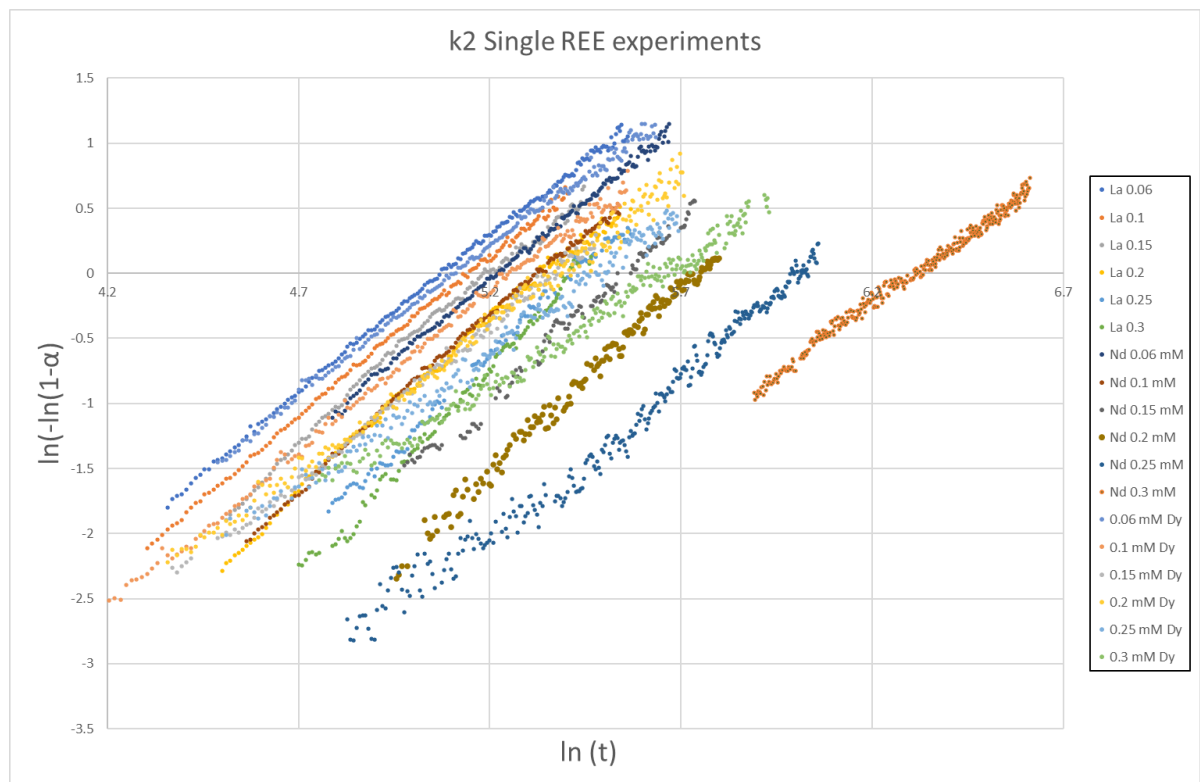
**Fig SI-1.** SEM picture showing the location of points of analysis displayed in Table SI-2.



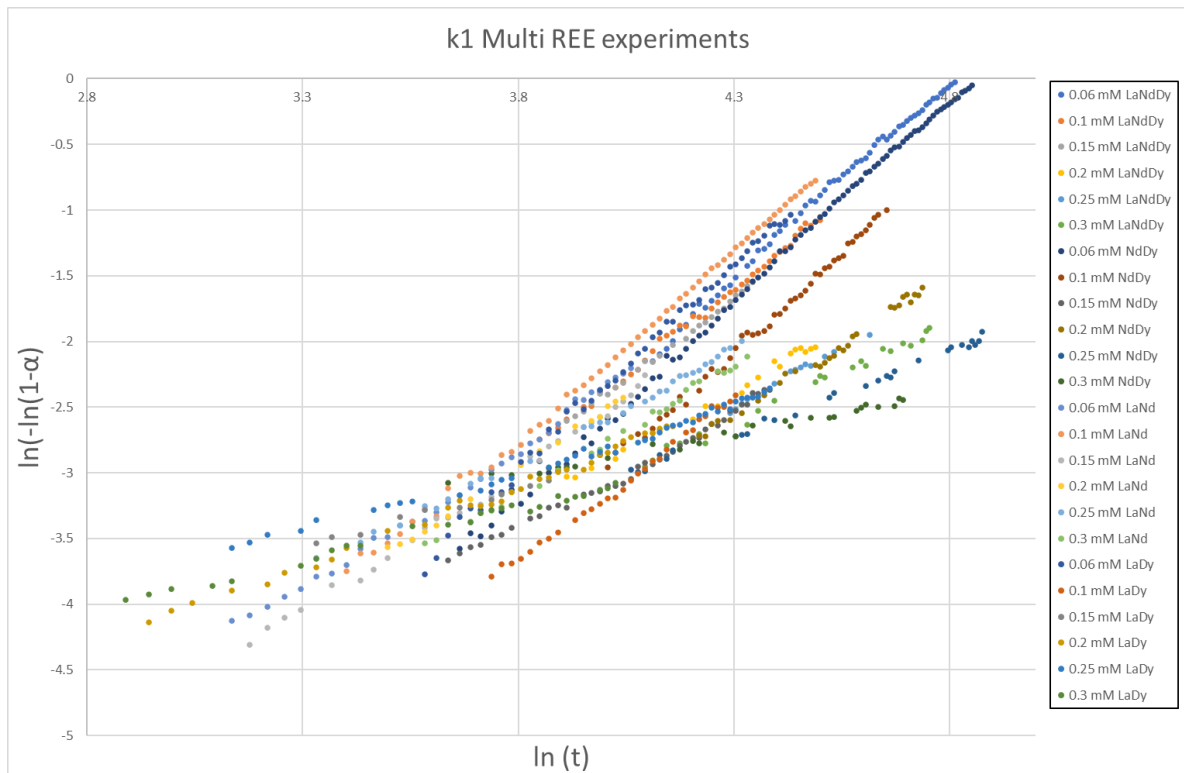
**Fig SI-2.** Graph showing the  $k_1$  of the single REE experiments.



**Fig SI-3.** Graph showing the  $k_2$  of the single REE experiments.



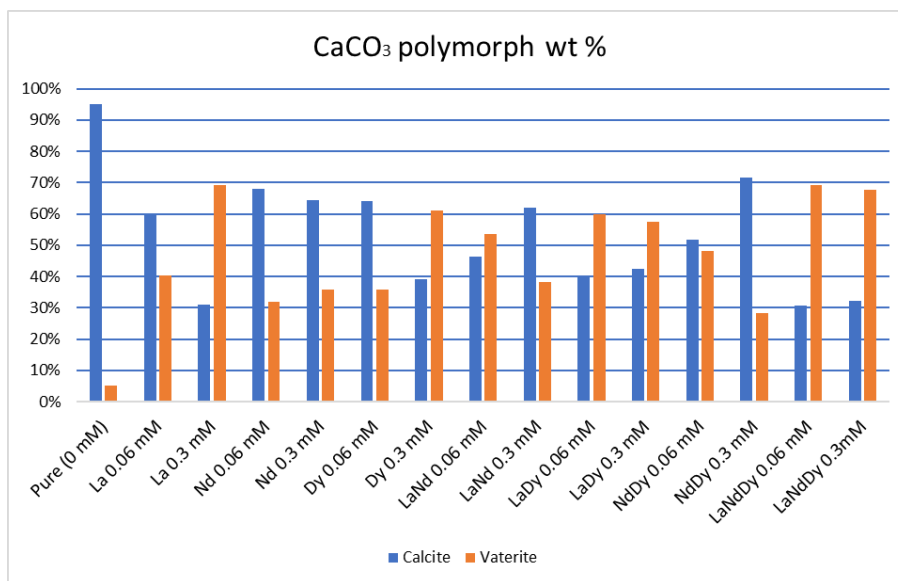
**Fig SI-4.** Graph showing the  $k_1$  of the multi REE experiments.



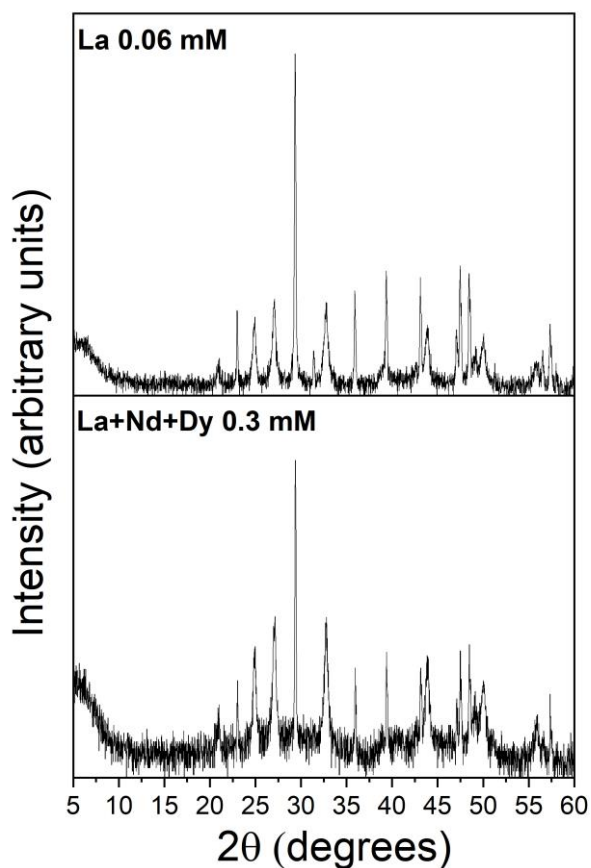
**Fig SI-5.** Graph showing the  $k_2$  of the multi REE experiments.



**Fig SI-6.** Graph showing the wt% of calcite and vaterite obtained in all the single and multi-REEs experiments.



**Fig SI-7.** XRD patterns showing two samples in which it is possible to identify the absence (La 0.06 mM, above) and the presence (La+Nd+Dy, below) of humps that correspond consistently to poorly-ordered precursor phases.



**Fig SI-8.** Powder XRD patterns of the pure system (0 mM REEs) and of the experiments in the presence of La+Nd+Dy both at low (0.06 mM) and high (0.3 mM) concentration. The small square next to the pure system pattern is a zoom between 20 and 35  $2\theta$  degrees in order to show better the presence of the vaterite peaks.

