

Supplementary materials

Magnesium Coprecipitation with Calcite at Low Supersaturation: Implications for Mg-enriched Water in Calcareous Soils

Mostafa Abdollahpour ^{1,†}, Frank Heberling ^{2,*}, Dieter Schild ², and Rasoul Rahnemaie ^{1,*}

¹ Department of Soil Science, Tarbiat Modares University, Tehran P.O. Box 14115-336, Iran;
m.abdollahpour@modares.ac.ir

² Institute for Nuclear Waste Disposal, Karlsruhe Institute of Technology, Hermann-von-Helmholtz Platz 1,
76344 Eggenstein-Leopoldshafen, Germany; dieter.schild@kit.edu

* Correspondence: frank.heberling@kit.edu (F.H.); rahnemaie@modares.ac.ir (R.R.)

† Visiting Scientist at Institute for Nuclear Waste Disposal, Karlsruhe Institute of Technology,
Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen, Germany.

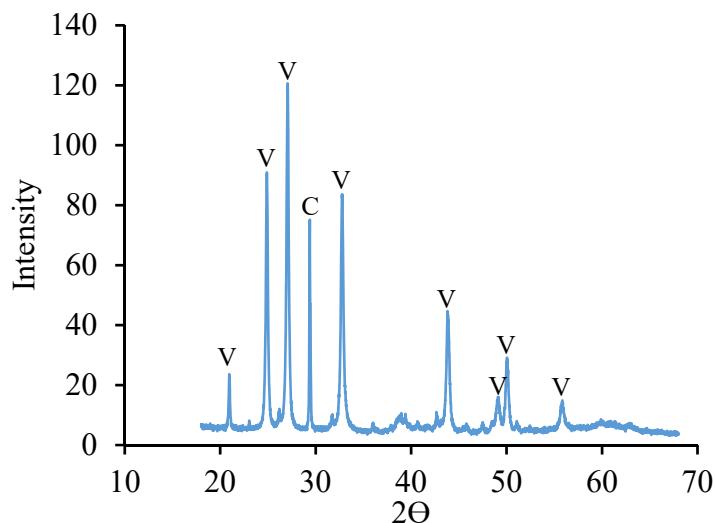
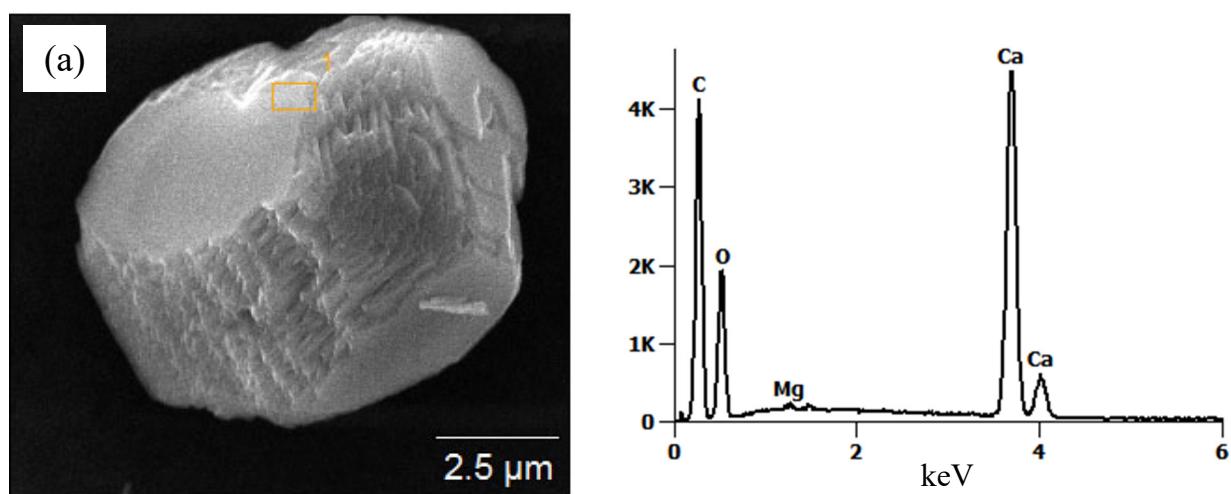
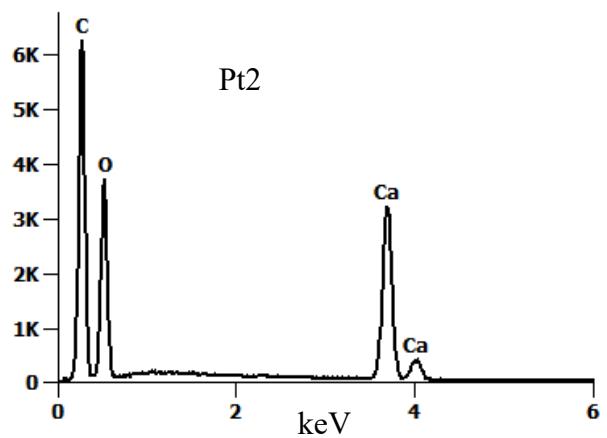
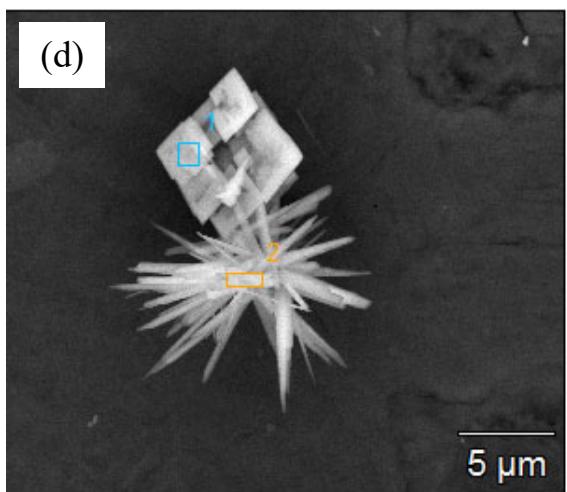
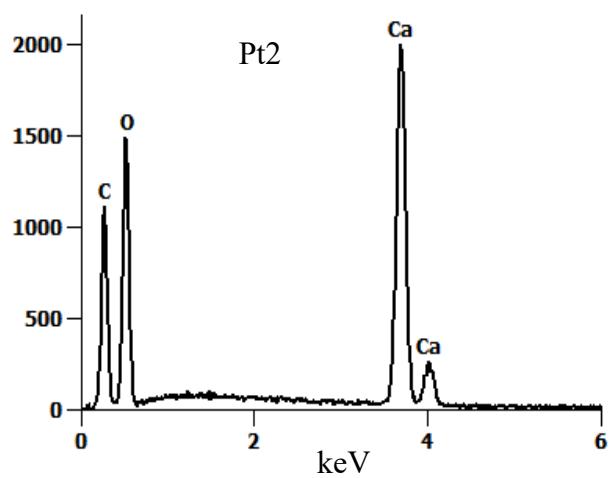
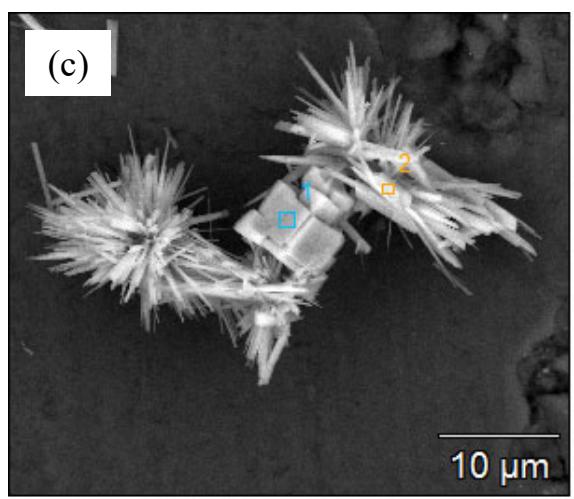
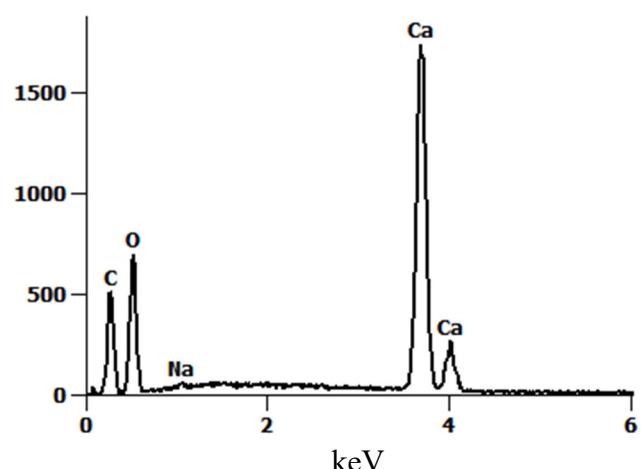
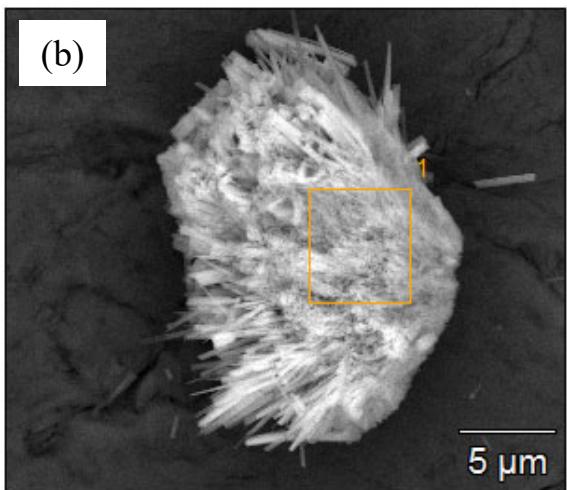


Figure S1. X-ray diffraction pattern (XRD) of the synthesized vaterite. V and C denote the diffraction peaks assigned to vaterite and calcite, respectively. Rietveld analysis shows that about 98% of the solid phase is vaterite. The remaining 2% are calcite.





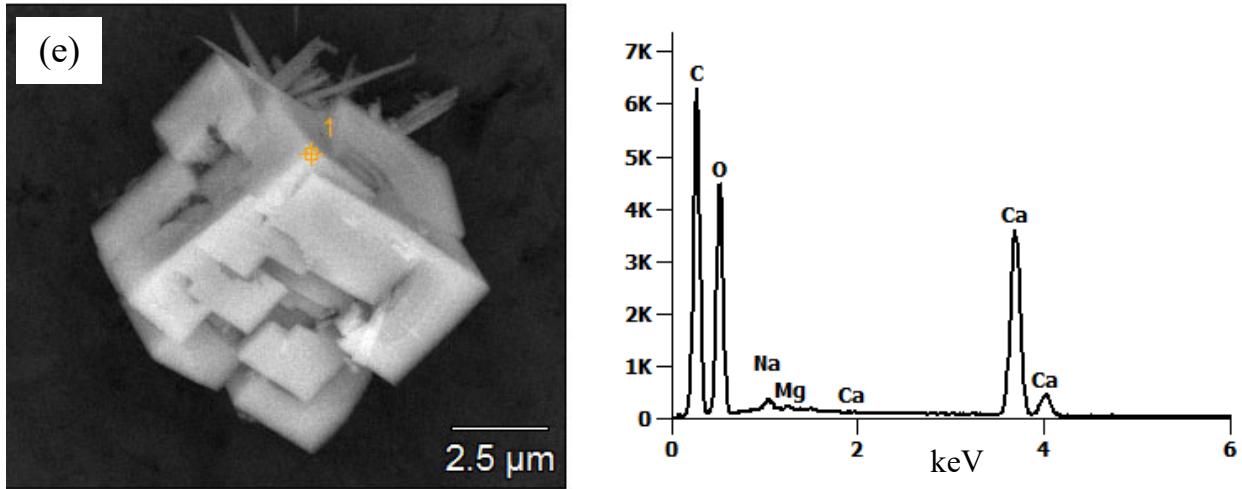


Figure S2. Selected scanning electron microscopy (SEM) images and their corresponding EDX analyses results of precipitated solids during transformation of vaterite to Mg-calcite and/or aragonite for an average actual pH of 8.8. Mg to Ca ratios are (a) 0.2, (b) 1, (c) 2, (d) 5, and (e) 10. EDX analyses results for Figures (c) and (d) are related to the point 2. At lower Mg to Ca ratio, where the Mg incorporation is relatively high, more EDX measurements were performed. For instance, at Mg to Ca ratio of 0.2, more than 45 surface points of Mg-Calcite were analyzed. At higher Mg to Ca ratios, less surface points were analyzed.

Table S1. The ionic composition of solution phase and X-ray diffraction results of the precipitated solids precipitated in contact with 0.2 and 1 g/L of kaolinite and bentonite clays and four magnesium (Mg) to calcium (Ca) ratios. The acronym 'TIC' denotes total inorganic carbon.

Clay (g/L)	Mg to Ca ratio	Initial Mg (mmol/L)	Mg	Ca	TIC	Removed Mg	Mg	Mg-calcite	Aragonite	Vaterite
			(mmol/L)			(mol/kg)		%		
			Supernatant	Solution	Solid					
Kaolinite	0.2	0.5	0.42	0.83	1.52	0.10	0.05	82	18	-
	1	2.5	2.46	0.83	0.99	0.05	0.02	6	94	-
	0.2	2	4.84	0.85	0.90	0.19	0.02	5	95	-
	5	12.5	10.79	0.89	0.96	2.05	0.02	3	97	-
Kaolinite 1	0.2	0.5	0.39	0.91	1.12	0.22	0.09	59	41	-
	1	2.5	2.46	0.94	1.24	0.09	0.04	5	95	-
	2	5	4.81	0.96	1.31	0.37	0.05	4	96	-
	5	12.5	10.82	0.99	2.07	3.35	0.04	7	93	-
Bentonite	0.2	0.5	0.38	0.83	1.05	0.15	0.12	66	44	-
	1	2.5	2.43	0.86	1.14	0.08	0.09	6	68	26
	0.2	2	4.81	0.87	1.20	0.22	0.10	4	72	24
	5	12.5	10.70	1.00	1.34	2.15	0.12	4	39	57
Bentonite 1	0.2	0.5	0.41	0.64	0.98	0.18	0.17	7	8	85
	1	2.5	2.32	0.78	1.05	0.37	0.33	3	3	94
	2	5	4.65	0.83	1.07	0.70	0.41	3	3	94
	5	12.5	10.54	1.01	1.30	3.92	0.48	1	-	99