Electronic Supplementary Material (ESI) for Environmental Science: Nano.


# Supporting Information of:

## Mechanisms limiting the release of $TiO_2$ nanomaterials during photocatalytic cement alteration: the role of surface charge and porous network morphology

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**Keywords**: Life cycle, exposure, pore throat size, micro and nano X-ray computed tomography (micro and nano-CT), 3D imaging.

**Description of sample preparation of altered cement for X-ray analysis (XRD, micro-XRF, Micro-CT and Nano-CT**

7-day altered cement pellets were coated within epoxy resin (Araldite AY 103 mixed with hardener Hy 956) to preserve the structure of the very porous and friable altered surface layer. Embedded leached cement pellets were cut perpendicularly to the cement surface into a slice of 10 × 10 × 5 mm for micro-XRF imaging and stick of 0.4 × 0.4 × 15 mm for nano-CT using a precision saw (IsoMET 4000, Buehler). Obtained slice/ stick are cross-sections of the sample including three layers: the resin, the altered layer at the cement surface and the unaltered core. For XRD analysis altered cement pellets were not coated with Araldite. After 7 days of leaching, altered cement pellets were dried under an N2 atmosphere to prevent secondary surface carbonation. Then the altered layer was separated from the unaltered core by a smooth polishing of the pellet surface (using a sanding paper with a grain size of 200 µm).

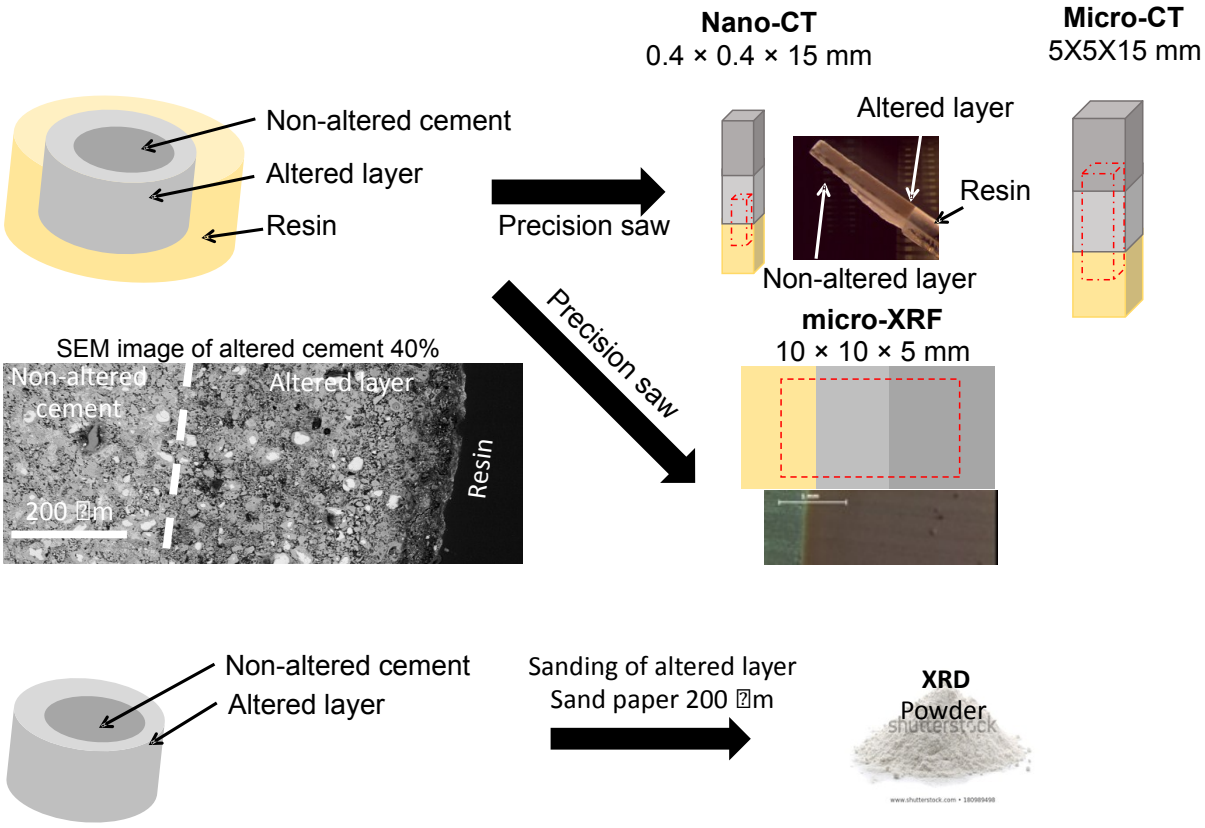


**Figure S1: Schematic view of altered sample preparation for X-ray analysis ( XRD, micro-XRF, Nano-CT and Micro-CT)**

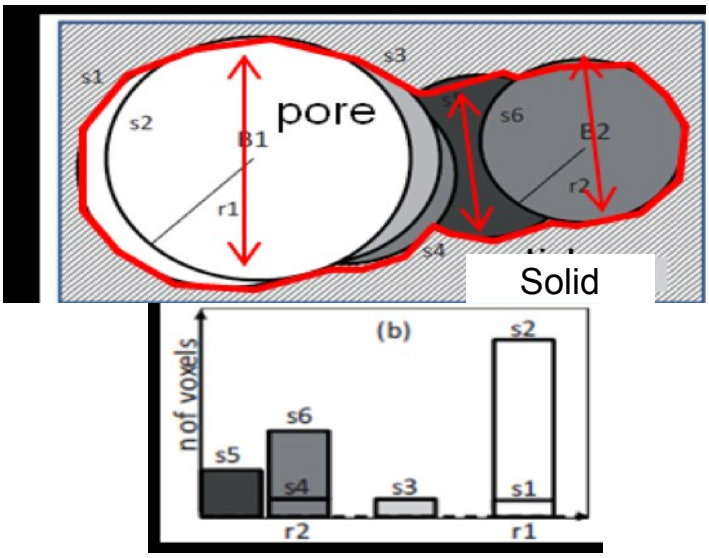


**Figure S2: Schematic view of the I-Morph operator to obtain the granulometric volume distribution of the void phase**

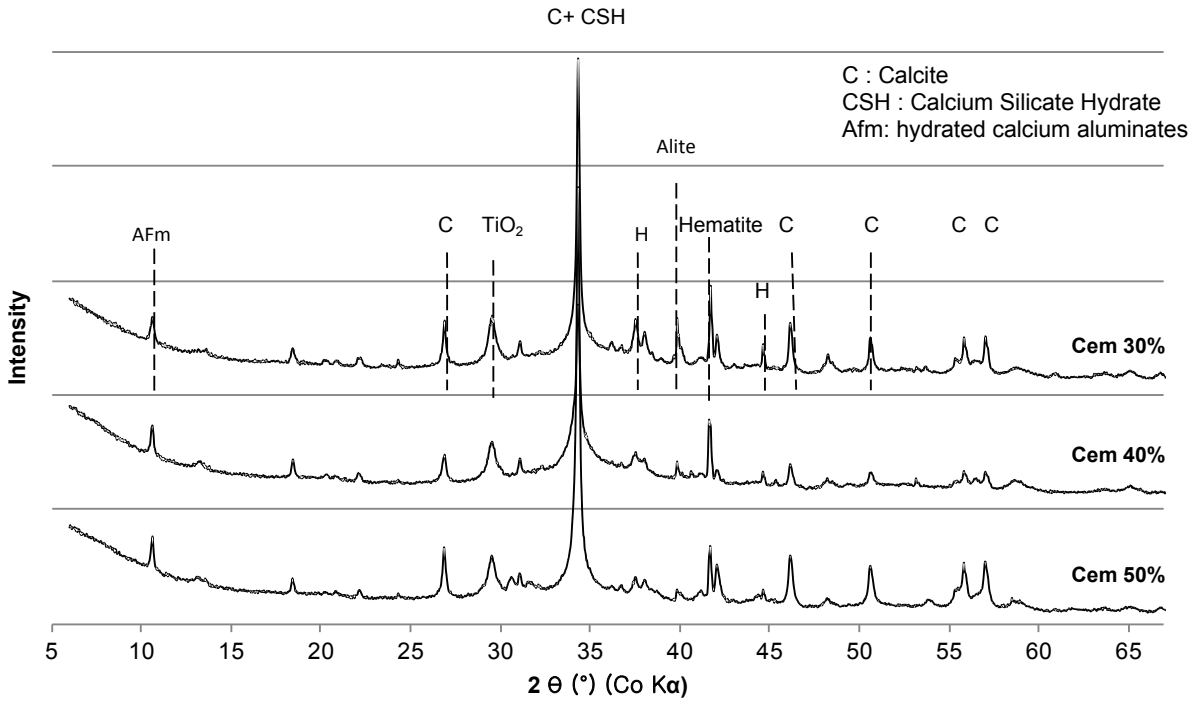


**Figure S3: X-ray diffraction (XRD) patterns of cement 30%, cement 40% and cement 50% of the first 100 microns of the altered layer. Hematite is coming from the sand paper used to remove the very altered layer of cement pellets.**

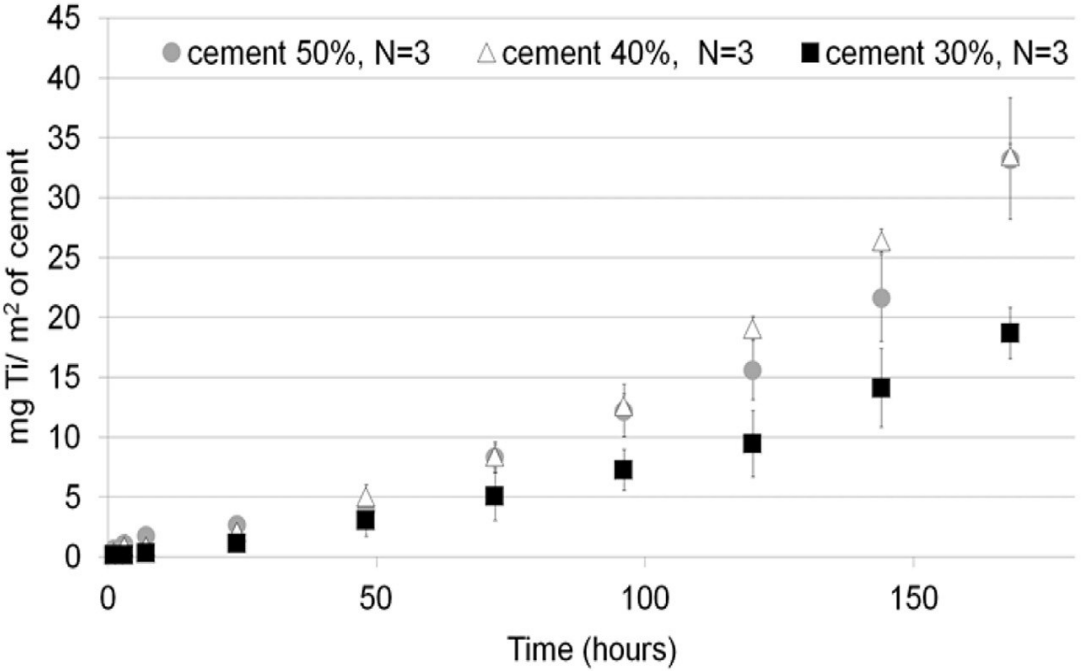


**Figure S4: Total amount of particulate Ti released during leaching of hardened cement 30, 40 and 50% over a time course. Released amounts are normalized by the cement external surface (extracted from[1])**

**Anydrous photocatalytic cement and control cement chemical composition**

| wt.% | OM | LOI | $Al_2O_3$ | CaO | $Fe_2O_3$ | $K_2O$ | MgO | $SiO_2$ | **$TiO_2$** | TOTAL |
|---|---|---|---|---|---|---|---|---|---|---|
| Photocatalytic cement | 1.88 | 1.70 | 5.05 | 65.19 | 0.34 | 0.06 | 0.68 | 23.21 | **2.85** | 101.06 |

**Table S1. Cement photocatalytic chemical composition (expressed as oxides in mass percentage (wt.%) measured by ICP-AES analysis after cement mineralization (alkaline digestion) (OM: organic matter and LOI: lost oxygen index). (extracted from[1])**

## Reference

1 N. Bossa, P. Chaurand, C. Levard, D. Borschneck, H. Miche, J. Vicente, C. Geantet, O. Aguerre-Chariol, F. M. Michel and J. Rose, *Environ. Pollut.*, 2017, **220**, 1160–1170.