Atomic and vibrational origins of mechanical toughness in bioactive cement during setting

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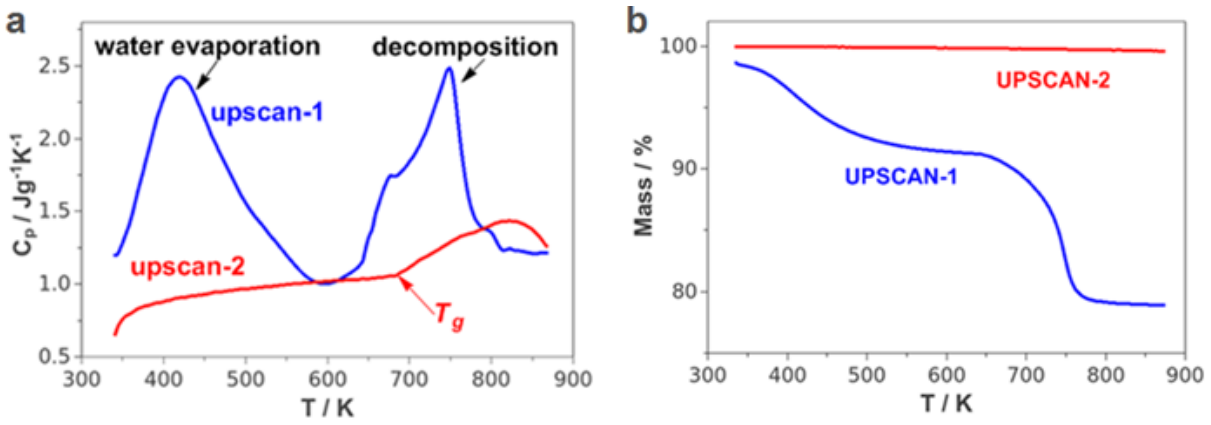
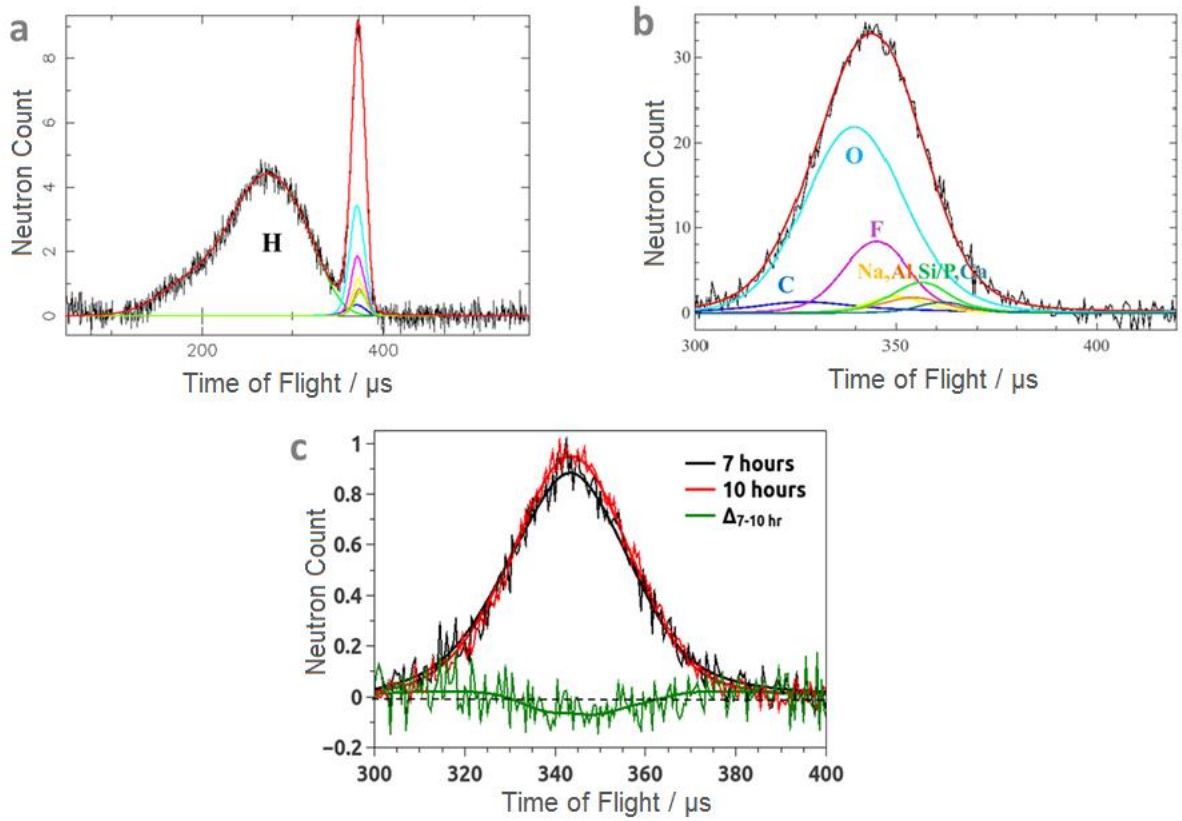
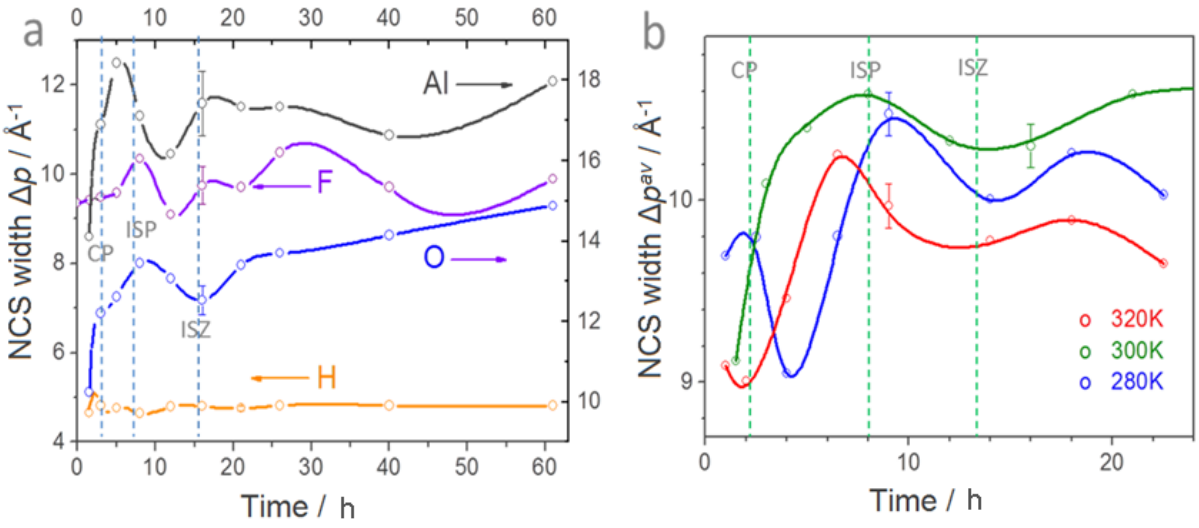


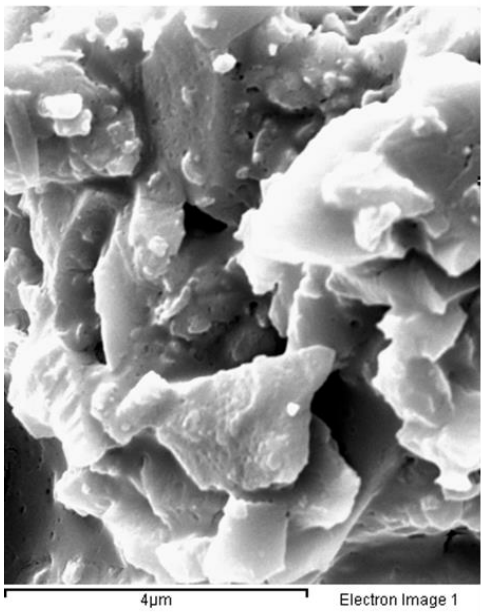
Supplementary Figure 1 | a: Isobaric heat capacity (C_p) (**a**) and mass change (**b**) as functions of temperature for the GIC sample after 62 hours setting, showing release of water and organic components.



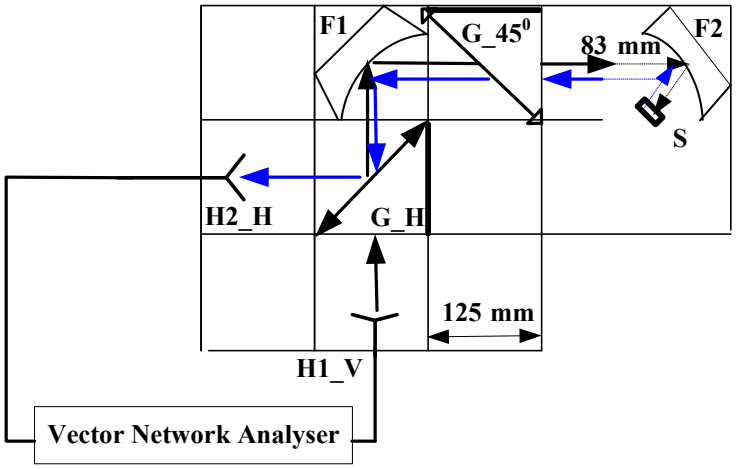
Supplementary Figure 2 | **a**, Example of forward scattering ToF data deconvoluted into elemental contributions by mass, each weighted by the stoichiometry. **b**, Corresponding backscattering peaks. **c**, NCS profiles (raw and fit data) of the total cement envelope at 7 and 10 hours, after initiation of setting; difference spectrum (raw and fitted data) is shown in green.



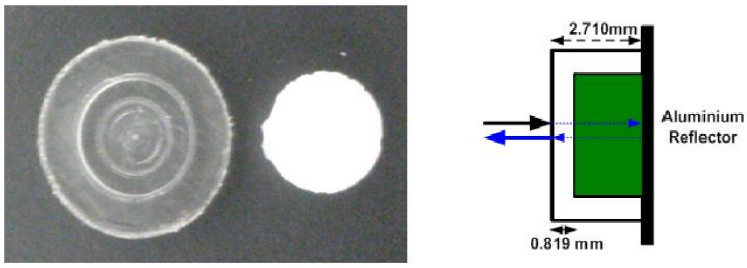
Supplementary Figure 3 | **a**, Elemental NCS peak widths Δp_i for H, O, F and Al. **b**, Average NCS peak widths $\Sigma_i c_i \Delta p_i$ for setting at 280 K, 300 K and 320 K, where c_i is the elemental atomic fraction. CP-coupling point, ISP-initial setting point, ISZ-intermediate stress zone; corresponding to early composite setting stages from Fig. 3.



Supplementary Figure 4 | SEM image of cement glass particles showing fractured surfaces.



Supplementary Figure 5 | Schematic diagram of the quasi-optical transmissometer. H1 and H2 denote a pair of corrugated feed-horns transceiver and the latter capital letter V and H present the linearly-vertical and horizontal polarised electric fields, respectively; F1, is an ellipsoidal reflector with focal length 250 mm and F2, a spherical mirror with focal length 83 mm; G_H presents a wire-grid with horizontal polarization and G_45^0 stands for a wire-grid with 45^0 polarization and S is the sample under test.



Supplementary Figure 6 | (left) Real TPX® cap and GIC; (right) the schematic plot of TPX® cap and the samples under the test are fully filled in the green area.