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Tracking Setting Dynamics in Cementitous Materials

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Despite increasing demands for improved biomaterials, rational design and optimisation remains incomplete. Glass ionomer cements (GICs), widely used in dentistry and orthopaedics (Fig.1), offer apposite examples, combining glass brittleness with polymer ductility - but a resultant composite insufficiently tough for load-bearing applications. Using a combination of *in situ* spectroscopies, we have discovered how toughness at the atomic level varies non-monotonically during setting. Transmission Electron Microscopy (TEM) and Differential Scanning Calorimetry (DSC) identify phase separation, the latter also evidencing high thermal stress in the glass component. Neutron Compton Scattering (NCS) identifies a setting point, where decreasing toughness momentarily recovers. Concurrent Structure Factor variations point to associated weaknesses developing at the glass-matrix interface, while Coherent Terahertz Spectroscopy reveals the coupling point where both components engage. Quantum chemical calculations modelling the hybrid interface, predict the collective vibrations that drive coordination modifications governing toughness.

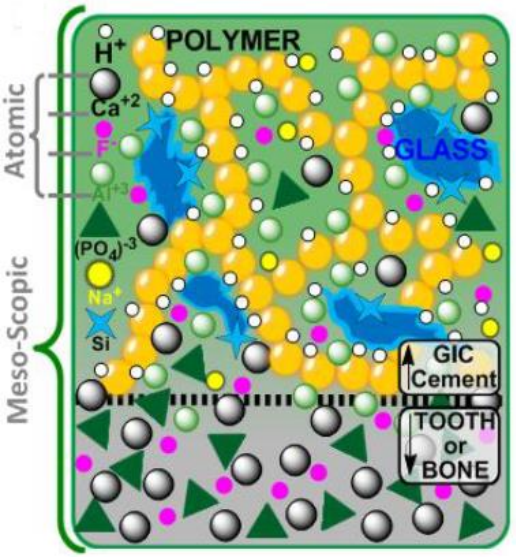

Fig.1 Illustration of the mutli-scale structure and ion-exchange interface of bioactive glass-cement

The talk covers the results on glass cements, with a focus on the insight afforded by these correlated studies which may well help to open the way to design new generation composite materials with optimal practical and clinical performance.