Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

In situ synchrotron X-ray diffraction reveals the disassembly-organisation mechanism of germanosilicate zeolites in HCl vapour

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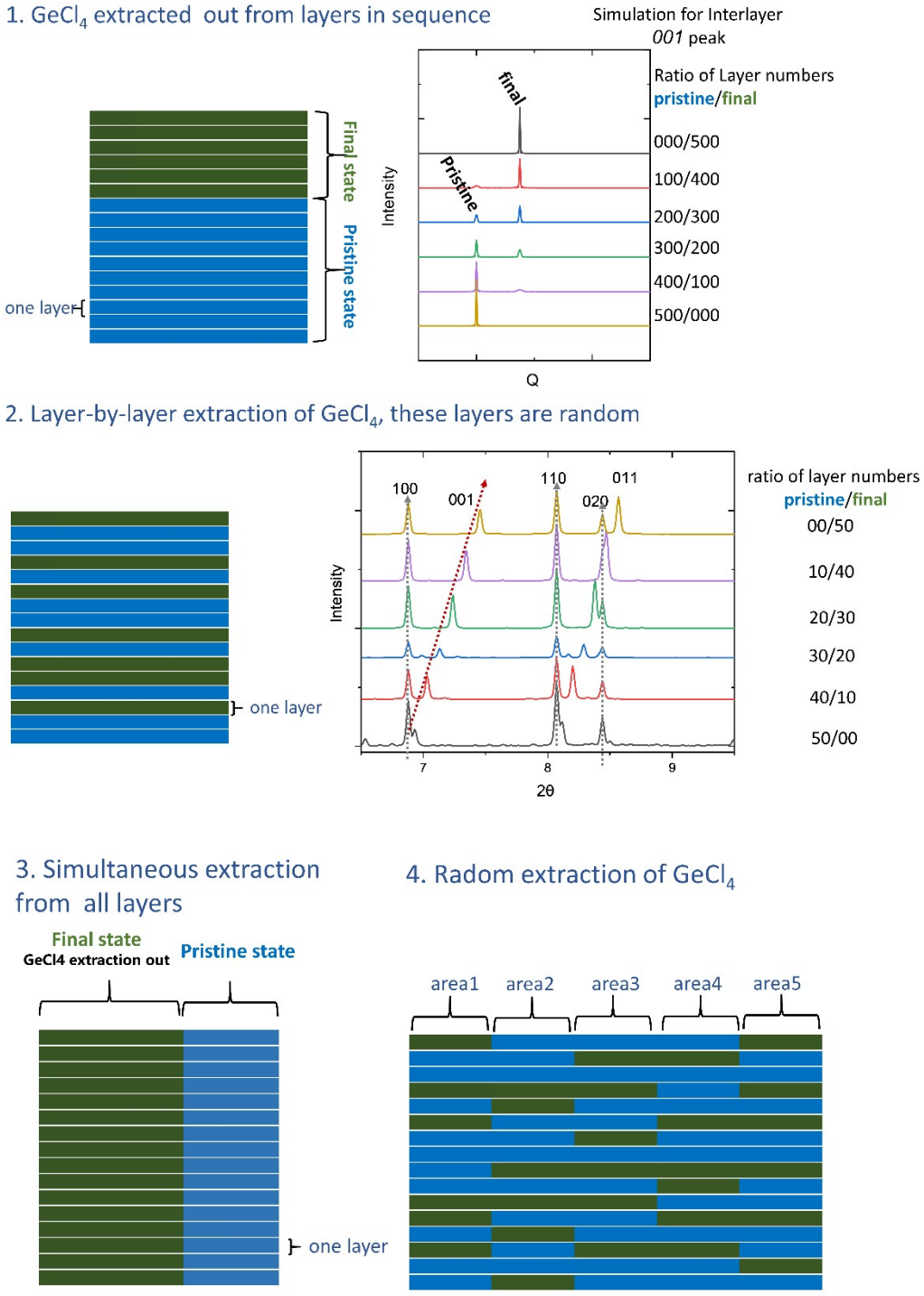

Fig. S1 Four models for the extraction of $GeCl_4$ process are proposed. The lattice parameters of the pristine state (blue) and final state (green) are preset as c = 12.9 Å and 12.0 Å, respectively, together with a = 13.0 Å, b = 21.2 Å in orthorhombic unit cells. The XRD patterns in Model 1 are generated from GenX software, while Model 2 was from VESTA.

In the disassembly step, the completion of hydrolysis involves the break of four Ge-O bonds. For three zeolites, fast loss of intralayer diffraction peak intensities and further disappearance of peaks when contacting with the acid vapour happened in nearly 1 min, while the interlayer distances of IWR and UOV did not significantly change at this time. This indicates that the diffusion of acid vapour into the zeolite channel and the initiation of hydrolysis are very fast, not through the layer-by-layer hydrolysis, otherwise, we would observe two sets of diffraction patterns (Model 1 and Model 3). While Model 4 with fully disordered structures in all directions would lead to more complicated changes of the diffraction peaks, not as the experimentally observed smooth shifts in d spacings. Therefore, Model 2 is most likely to occur in the disassembly and organisation steps.