

diffraction data, this conference.

[2] A.Falenty et al., Stop-and-go *in-situ* tomography of dynamic processes –gas hydrate formation in sedimentary matrices, this conference

[3] Klapp et al. (2010), *Earth Planet. Sci. Lett.*, 299(1-2), 207-217, doi: 10.1016/j.epsl.2010.09.001.

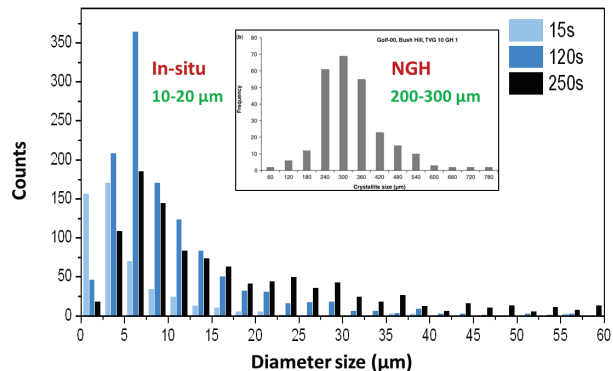


Figure 1. CSD of growing xenon hydrates after 15, 120 and 150 s. Insert shows the considerably larger CSD of a natural GH from Gulf of Mexico [3] indicative of appreciable coarsening of natural samples.

Keywords: In-situ, Crystallite Size Distribution, X-ray Dffraction, Gas Hydrates

MS17-P2 In-situ single crystal XRD study of absorption and desorption of CO₂ in zeolite Y

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X-ray diffraction methods in general allow only a limited chemical selectivity. Structural information on a subset of atoms is here obtained by modulating the stimulus supplied in situ on a crystal thus extracting structural information from the changing part of the scattering density within the overall crystal structure. Single crystal XRD data were collected in situ on a zeolite Y, in which CO₂, acting as active species, is desorbed upon heating. After out gassing the single crystal sample, anchored in a capillary, CO₂ was introduced in the capillary and the temperature modulated to obtain adsorption and desorption of the CO₂. In this way it has been possible to determine the sites where CO₂ is absorbed, its variations in occupancy and the motions between the sites. The cell parameter of the zeolite was found to decrease while increasing the temperature as CO₂ was desorbing, leaving the channels. It was then possible to determine the overall diminution in the occupancy of CO₂ while increasing the temperature and the shift of CO₂ moieties between the sites upon absorption and desorption.

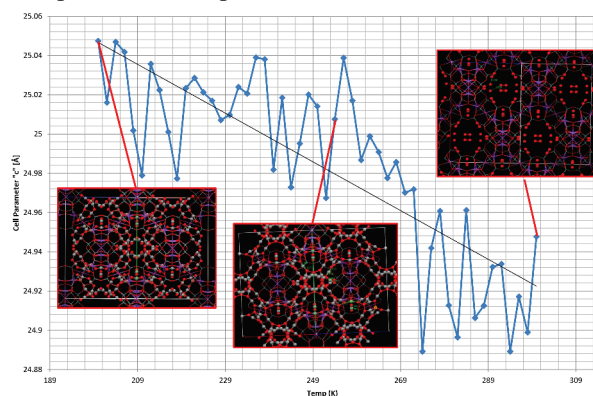


Figure 1. Cell parameter of Zeolite Y versus temperature and structures at selected temperatures.

Keywords: X-ray Single Crystal Diffraction, Chemical Selectivity, Substructure refinement, Modulation Enhanced Techniques, Fourier Filtering, Zeolites, Gas Adsorption.