Zeolites Gismondine and Li-ABW under Pressure: Synchrotron XRPD and MD Simulations

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The response to compression of the zeolites gismondine and of LiABW were explored by synchrotron X-ray powder diffraction and ab-initio Molecular Dynamics simulations. Different pressure-transmitting media were used: silicon oil and propane-isopropane as non-penetrating media, and a water-methanol mixture as penetrating one. The applied pressure spans from room pressure to about 10 GPa. The data collection was performed at SNBL1 beamline at ESRF (Grenoble) using a wavelength of 0.7 Å and a MAR 345 (pixel size 100 mm) IP detector; the 2θ accessed range is 0 – 36°. The behaviour of the unit cell parameters as a function of pressure and the bulk modulus values were derived by processing the powder patterns. The ab-initio MD simulations, performed on the basis of the experimental cell parameters, provided the atomistic structural interpretation of the response of gismondine to compression.

Gismondine cell parameters regularly decrease and the P-induced modifications are reversible upon decompression. The bulk modulus calculated on the basis of the experiment performed with silicon oil is K_0= 63.8(2) GPa. The bulk modula derived for the three data sets collected on LiABW using different P-transmitting media are K_0= 68(2), 64.8(8) and 60(5) GPa for silicon oil, alcohol-water and pentane-isopentane, respectively.

Keywords: zeolites, high-pressure diffraction, Molecular Dynamics simulations