Structure refinement using precession electron diffraction tomography and dynamical calculations: application to pyroxene

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The precession electron diffraction (PED) technique originally developed for structure determination at a submicrometer scale in a TEM is usually combined with tomographic acquisition of 3D electron diffraction data (PEDT). Very recently, a full structure refinement method based on PEDT data and dynamical calculations of diffracted intensities has been successfully proposed [1]. We present some results concerning the application of this new method to the refinement of $(Mg,Fe)SiO_3$ pyroxene structures in order to determine the Fe^{2+} and Mg ordering on specific mixed sites of these structures of mineralogical interest. The refinement of 3D electron diffraction data against dynamical calculations enables the estimation of the (Fe,Mg) occupancies with a good precision, the refined values being closed to those deduced from XRD experiments at the grain scale. We will discuss on the accuracy and sensitivity of the method to experimental and computational parameters and on its potential application in the field of geothermometry using local analysis of terrestrial or extra-terrestrial pyroxene bearing rocks.