Zeolites are crystalline microporous aluminosilicate minerals with numerous industrial and scientific applications, including catalysis, preparation of advanced materials and nuclear processing. Transmission Electron Microscopy (TEM) is a very powerful technique to characterize the structure and composition of such materials at the atomic scale. For the case of cation exchanged zeolites, it is of crucial importance to determine the atomic positions of the cations in the zeolitic framework. Such knowledge enables one to understand and optimize the connection between the structure and the properties of the materials. Recently, high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) was used to image Ag cations in the LTA framework. HAADF-STEM images yield an intensity which scales with the atomic number Z and the thickness of the sample. Therefore, the Ag cations will appear with higher intensity in comparison to the elements in the zeolitic framework (Si, Al and O).

Unfortunately, zeolites are extremely sensitive to damage caused by the electron beam, especially in the case of a relatively low Si/Al ratio. The use of aberration corrected TEM at relatively low electron dose, however, does enable one to obtain high resolution images. Here, we combine monochromated, aberration corrected HAADF-STEM with a careful image analysis, the so-called template matching technique, in order to determine differences in the 3 dimensional positions of Ag cations present in FAU-X and FAU-Y. For both samples, which have an fcc structure, HAADF-STEM images were therefore acquired along the three main zone axes [100], [110] and [111] and compared with the results from X-ray diffraction (XRD). This is illustrated in Figure 1 and Figure 2 for the [110] zone axis. This enabled us to propose a 3D model for the atomic structure of Ag-exchanged FAUY and FAUX zeolites (Figure 3).

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Fig. 1: High resolution HAADF-STEM image of Ag exchanged FAU-X zeolite, acquired along [110]. The inset presents the results of the averaging procedure of the template matching, using 50 templates.

Fig. 2: a) Comparison between the averaged image and the XRD model (overlay) for the FAU-X along the [110] zone axis. Inconsistencies between the experimental image and the XRD model are indicated by yellow circles in Figure a. b) Comparison between the averaged image and the refined model (overlay).

Fig. 3: Proposed model for FAU-X sample, oriented along the [110], [100] and [111].