Application Note B-XRD1131

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B-XRD1131 - Structural characterization of zeolite by PDF analysis

Introduction

Zeolites, which are microporous aluminosilicates, have excellent properties, such as water absorption ability, ion exchange capacity, molecular sieving ability and catalytic ability. The crystal structure is composed of TO_4 tetrahedra (T = Si, Al) that share each oxygen atom to form n-membered rings. Although zeolites are basically crystalline solids, heating treatment (HT) collapses the crystal structure, turning them into amorphous solids. Rietveld refinement is generally used to characterize crystal structures, but it is not applicable to amorphous materials due to the broadness of the peaks, called halos. However, PDF analysis can derive structural information from amorphous material, thereby solving this problem.

Measurements and results

XRD measurement was performed for CHA (chabazite) type zeolite before and after the HT. Figure 1 shows XRD patterns corresponding to each condition. Since the XRD pattern before the HT has sharp peaks, it is a crystalline zeolite. On the other hand, the XRD pattern after the HT has some halos; therefore, it has changed to amorphous zeolite. To perform the structural analysis, PDF analysis was performed. The results are shown in Figure 2. The peak positions correspond to atomic distances r respectively. Before and after the HT, the peak intensity of the correlation distance of Si-O in 4-membered rings (Figure 3) decreased, while the peak intensity of the correlation distance of Si-O in 6, 8-membered rings did not change. Hence, it is presumed that the 4-membered rings collapse in the amorphous structure. Additionally, because the PDF pattern of zeolite is similar to the PDF pattern of SiO_2 glass, it is estimated that the amorphous structure of CHA is close to the glass structure.

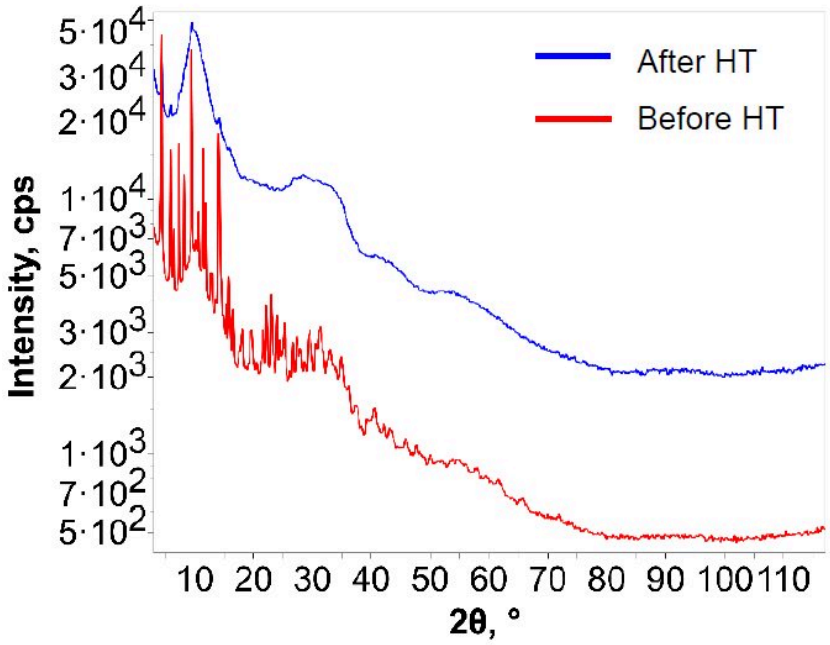

Figure 1: XRD patterns of zeolites before and after HT (Offset process was applied to "after HT" data)

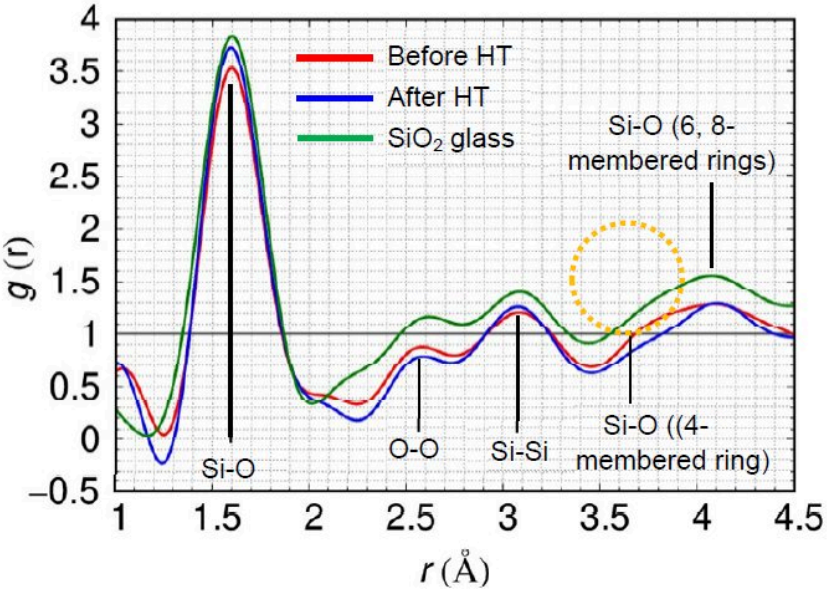

Figure 2: PDF patterns of zeolite before and after HT, and SiO_2 glass (Offset process was applied).

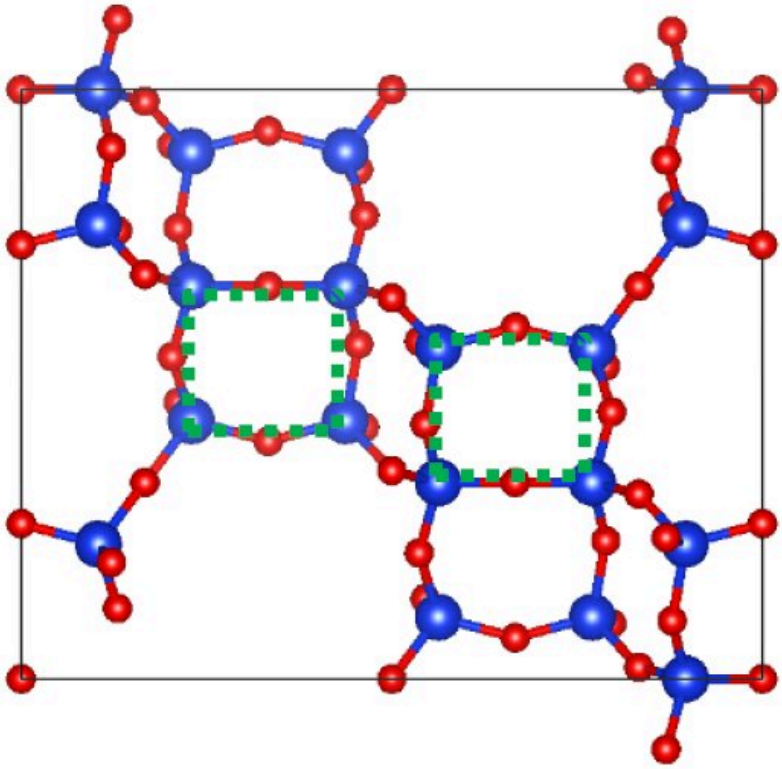

Figure 3: 4-membered rings of CHA (red ball: O, blue ball: Si, green frame: 4-membered ring).

Related products

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