Local structure of zeolite Beta from neutron diffraction

Inmaculada Peral, Robyn J. Accardi, Maria Martinez-Inesta, Thomas Proffen* and Raul F. Lobo
University of Delaware; Newark, DE 19716; Los Alamos National Laboratory*
email: lobo@che.udel.edu

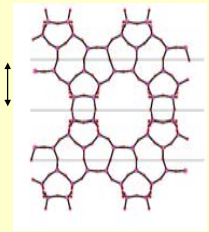
Motivation

Local structure of zeolite Beta

It is common to find stacking disorder in zeolites. This disorder is caused by the existence of more than one arrangement of the tetrahedra along one direction. Zeolite Beta is a good example of this type of materials.

Zeolite Beta has been extensively studied and its structure has been always described as the intergrowth of two polytypes (A and B). The aim of our work is the study of the local structure of zeolite from neutron diffraction using the Pair Distrution function.

Interlayer Distance=6.6Å



Zeolite Beta

Why using the Pair Distribution Function (PDF)?

Disorder in materials results in diffuse scattering which is of great importance in the characterization of the local structure. Unfortunately this diffuse scattering information is lost when performing a background correction of the Bragg diffraction pattern. Recently, researchers have been using the pair-distribution function (PDF) as a way to investigate the local structure of crystalline materials[1].

As the average structure of zeolite Beta is known[2], we expect that the study of the experimental PDF will provide a complete description of the structure of this zeolite. Moreover, the use of the PDF for zeolite Beta, which is a faulted zeolite will demonstrate whether the PDF may be useful when exiting stacking faults, which usually makes difficult the resolution of the structure.

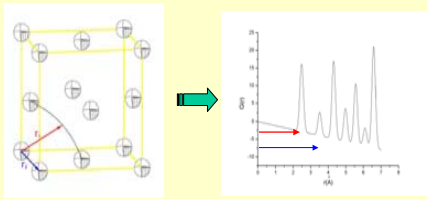
The PDF method

The PDF method is able to use data from the diffuse scattering as well as the Bragg diffraction[1]. The PDF is obtained from the powder diffraction data via a simple Fourier transform of the normalized intensity S(Q). In order to refine the experimental PDF one needs to calculate a PDF from a structural model.

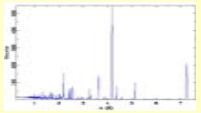
Simulated PDF

$$g(r) = \frac{1}{r}\sum\sum\left[\frac{b_i \cdot b_j}{\langle b\rangle^2}\delta(r - r_{ij})\right] - 4\pi r\rho_o$$

i, j = atoms
r_{ij} = distance between i and j
<b> = avg. scattering power of sample
ρ_0 = average number density

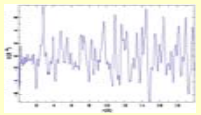


Experimental PDF



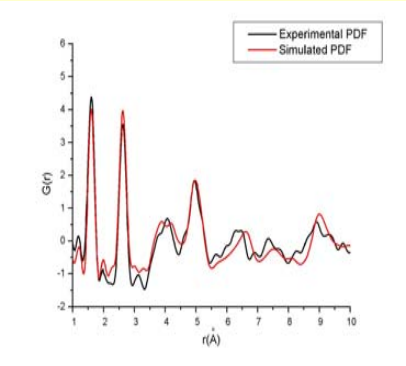
$$g(r) = 1 + \frac{1}{2\pi^2 r\rho_0}\int_0^\infty [S(Q)-1]\sin(Qr)Q\,dQ$$

Q = $4\pi\sin(\theta)/\lambda$ (elastic scattering)
S(Q) = normalized scattering intensity



Graphs taken from Dr. Billinge's group web page: www.totalscattering.org

Results



Experimental and simulated PDF plot shows that the published structural model describes the main features of the experimental PDF (peaks maximum position and intensity) although the complete description has not been achieved.

Conclusions

- It is possible to describe the main features of the local structure of zeolite Beta using the structural models from the literature.
- The refinement is not good enough, there are still differences between the simulated and the experimental PDF.
  This differences can be due to three possible causes:
  - -The existence of site defects of the Beta sample
  - -The low resolution of the instrument
  - -The structural model is not good enough to describe the local structure of zeolite Beta

Future work

We plan to measure at GEM (ISIS, UK) to get the best possible experimental Pair Distribution Function and get a better description of the local structure.

References
1. T. Egami, **Local Structure from Diffraction**, New York: Plenum, (1998) 1-23.
2. J. M. Newsam, et al., *Proc. R. Soc. Lond.* (1988) A420, 375.

Acknowledgements
Funding – NSF Zeolite Structure and NSF Career
Chris Benmore and Joan Siewenie at Argonne National Labs
Simon Billinge at Michigan State University