ESRF	**Experiment title: CRYSTAL STRUCTURE OF NEW ZEOLITE MATERIALS ERS-10 AND CR-1**	**Experiment number**: CH-1326
Beamline: BM01B	**Date of experiment**: from: 21.09.2002 to: 23.09.2002	**Date of report**: 21.02.2003
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Report:

Zeolites are crystalline microporous aluminosilicates with frameworks based on a three-dimensional network of corner-sharing TO_4 (T = Si, Al) tetrahedra. A zeolite framework can be described as a regular assembly of finite (Secondary Building Units, SBUs) or infinite building units (Periodic Building Units, PerBUs). These PerBUs are layers or chains, which stack in 1 or 2 directions to build a regular 3D structure. However, when two or more stacking modes are possible, the same PerBUs gives rise to different regular 3D structures as well as to disordered intermediates arising from the deviation of the stacking sequence from the periodic ordering, the most notable examples are ZSM-11 and Beta zeolites. The stacking faults are manifested by anisotropic broadening of a selected class of reflections peaks in powder diffraction patterns. Recently Carluccio *et al*. have reported the synthesis of the new ERS-10 zeolite whose XRD pattern is characterized by the typical features of an intergrowth material [1]. Preliminary structural characterization, indicated that the XRD pattern of ERS-10 is closely related to that of EU-1 (IZA code EUO) [2]. The aim of this study is the complete structural characterization of zeolite ERS-10 using the DIFFaX computer program [3].
CR-1 is a new zeo-type material, whose structure was unknown until now; unfortunately no single crystal suitable for single crystal analysis is available. The goal of the present experiment was to obtain an *ab-initio* structure model for this zeolite using high resolution powder pattern.

Experimental

Powder diffraction data were collected at the SNBL B station (BM01B) whose very high resolution powder diffractometer is equipped with six detectors and Si (111) analyzer crystals before them. The powder patterns were collected from 1 to 50° 2-theta; the wavelength employed was set to 0.79982 Å. An effective step size of 0.005 ° was used in rebinning the continuous –made-collected data. The counting time was optimized for each data collection in order to collect with good counting statistics the very weak reflection at high angle.

Results

The first step for the complete structure elucidation of zeolite material ERS-10 was the identification of the PerBUs present in the ordered structures and, to do that, we focused the attention on gottardiite [4], the natural counterpart of NU-87. The PerBUs identified in this structure were defined as layer I and layer II and introduced in the DIFFaX simulations. Several trials were performed adopting different layer-to-layer stacking probabilities and the results of each trial were evaluated by comparing the powder pattern calculated with DIFFaX with the synchrotron powder diffraction pattern of calcined ERS-10.

The basic features of the calcined ERS-10 synchrotron powder pattern are very satisfactorily reproduced, as reported in figure 1.

What emerges from this work is that ERS-10 is really an intergrowth of NON, EUO and NES zeolites, a conclusion supported by the fairly good agreement between the simulated and the experimental patterns.

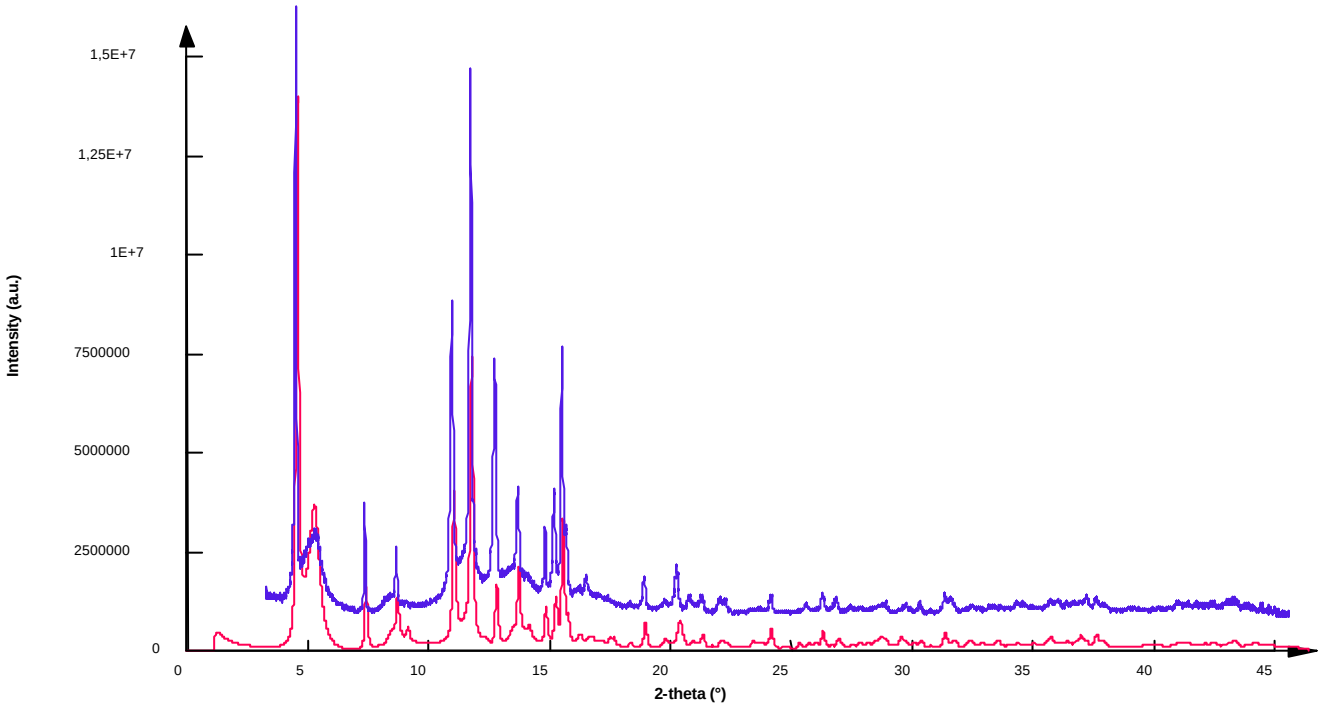

Figure 1: Show the good agreement between experimental powder pattern (blu line) and simulated one (red line).

The high resolution powder pattern of the as-synthesized form of zeolite material CR-1 was auto-indexed using the programs TREOR and DICVOL. The result was the same unit cell with parameters a = 10.56 Å, b = 13.97 Å c = 7.41 $\alpha = 90°$ $\beta = 97.96°$ $\gamma = 90°$. The symmetry proposed for zeolite CR1 was monoclinic and the possible space groups were the centrosymmetric $P2_1/m$ or the non-centrosymmetric one, $P2_1$.

Attempt to clarify the framework structure of this new zeolite material is still been in progress.

References

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